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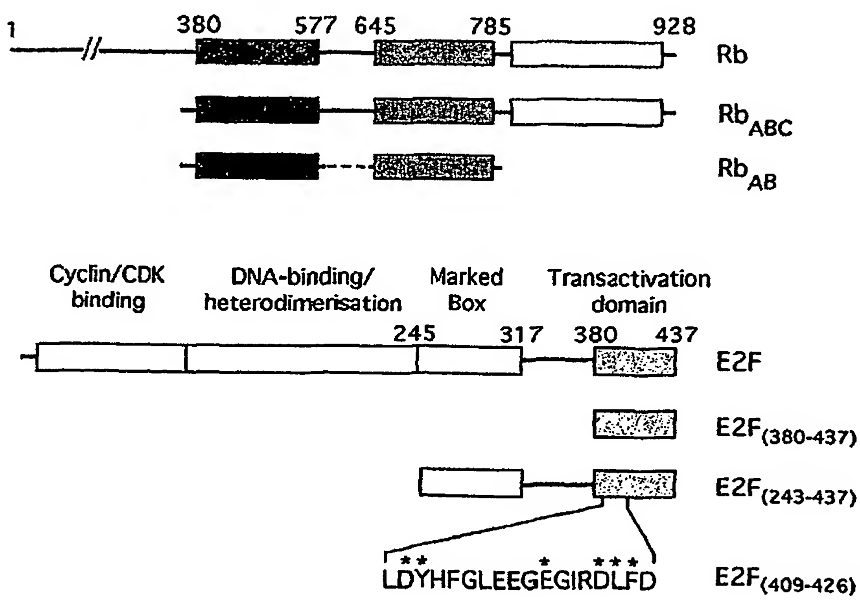

(57) Abstract: The present invention provides the crystal structure of pRb/E2F$_{(409-426)}$ as well as uses of the structure in identifying agents which modulate the binding between pRb and E2F and/or a pRb/E2F$_{(409-426)}$ complex, and thus are useful as pharmaceutical agents in the prevention or treatment of proliferative diseases.

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STRUCTURE OF A COMPLEX OF RETINOBLASTOMA PROTEIN BOUND TO E2F, AND USES THEREOF

The present invention relates to the crystal structure of pRb/E2F$_{(409-426)}$ as well as uses of the structure in identifying agents which modulate the binding between pRb and E2F and/or a pRb/E2F$_{(409-426)}$ complex, and thus are useful as pharmaceutical agents in the prevention or treatment of proliferative diseases.

The retinoblastoma tumour suppressor protein (pRb) regulates the cell cycle, sponsors differentiation and restrains apoptosis. Dysfunctional pRb is thought to be necessary for the development of most human malignancies.

pRb controls the cell cycle and apoptosis by acting as a negative regulator of transcription. It is now established that the growth-inhibitory effects of pRb are dependent on its regulation of the E2F family of transcription factors whose activity is necessary for the expression of genes involved in the G1 to S transition of the cell cycle and DNA replication. The transcriptional repression exerted by pRb over E2F responsive promoters involves at least three, distinct mechanisms. By binding to the transcriptional activation domain of E2F, pRb prevents it from recruiting components of the transcriptional apparatus and, once tethered to E2F promoters, pRb interacts with, and represses, other nearby transcription factors. Finally, pRb recruits protein factors to E2F promoters, such as histone deacetylases (HDACs) and histone methyltransferases (HMTases) that negatively regulate transcription by altering chromatin structure.

In addition to regulating entry into S-phase, it is thought that pRb is important in protecting differentiating cells from apoptosis. Certainly in many types of tissue, loss of pRb leads to apoptosis. This and other data has led to a model whereby the anti-apoptotic activity of pRb is mediated by its repression of certain E2F-dependent promoters. Unrepressed E2F is able to drive apoptosis by both p53-dependent and p53-independent mechanisms.

Although inactivation of the pRb pathway is thought to be widely involved in cellular transformation, there are examples of tumours where over-expression of functional pRb appears to be detrimental to successful clinical treatment. For example, adenocarcinoma of the pancreas is the fifth most common cause of cancer-related death in the Western world. It is particularly resistant to currently available forms of chemotherapy and radiation therapy. It is thought that this malignancy is able to evade apoptosis induced by treatment with chemotherapeutic drugs because of over-expression of pRb. It seems plausible that the protective effect of pRb over-expression against apoptosis is mediated by E2F. By blocking transcriptional activation by E2F, over-expression of pRb appears to render pancreatic cancer cells insensitive to chemotherapy.

As many of the anti-tumourigenic properties of pRb are mediated by its regulation of the E2F transcription factors, it would be beneficial to have a crystal structure of the pRb-binding fragment of E2F ($E2F_{(409-426)}$) in complex with the tumour suppressor protein. Such detailed knowledge of the molecular interactions between E2F and the A/B interface of pRb would enable the development of compounds that bind to pRb and inhibit complex formation. Such a compound, administered in parallel with conventional chemotherapy, would offer a means of enhancing treatment of proliferative diseases such as pancreatic cancer and perhaps related diseases.

Accordingly, the present invention provides the crystal structure of the primary pRb-binding fragment of E2F ($E2F_{(409-426)}$) in complex with the tumour suppressor protein pRb. The structure shows how $E2F_{(409-426)}$ binds at the interface of the A and B domains of the pocket of pRb making extensive interactions with conserved residues from both.

In order to address the regulation of the E2F transcription factor by pRb, the present inventors have determined the crystal structure of the complex of pRb_{AB} bound to the

minimal binding region of E2F, namely E2F$_{(409-426)}$. The structure has important implications for the understanding of pRb/E2F function. The studies have quantified the contribution of the principal interaction made by E2F through residues 409-426 with pRb as well as that of a secondary interaction involving the marked box region of E2F. In both cases these interactions are with the pocket region of the tumour suppressor protein pRb.

The analysis of the crystal structure of pRb/E2F$_{(409-426)}$ suggests that E2F$_{(409-426)}$ acts as a sensor of the structural integrity of the pRb pocket. Accordingly, cells in many tissues should be protected against deleterious mutations in pRb because they will sponsor increased E2F transcriptional activation, and thus apoptosis. It seems particularly intriguing, therefore, that all tumour derived pRb mutants fail to bind to E2F suggesting that an intense selectionary pressure operates in many types of tissue in favour of cells which harbour defects in apoptosis once they have lost normal pRb function. Perhaps the most notable exception to this process occurs in retinal cells, which are able to survive for some time with loss of pRb without acquiring other genetic alterations. Indeed, it has been suggested that these particular cells are distinguished by their ability to acquire survival signals from neighbouring cells and thus give rise to the eponymous retinoblastomas.

According to a first aspect, the present invention provides a crystal structure of the pRb/E2F$_{(409-426)}$ complex, characterised by the atomic co-ordinates of Annex 1.

Preferably the interactions between E2F$_{(409-426)}$ and pRb comprise one or more of the following interactions:

E2F$_{(409-426)}$ residue	**pRb residue**
Leu$_{409}$	Lys$_{548}$
Tyr$_{411}$	Glu$_{551}$

$E2F_{(409\text{-}426)}$ residue	pRb residue
Tyr_{411}	Ile_{532}
Tyr_{411}	Glu_{554}
His_{412}	Arg_{656}
His_{412}	Lys_{653}
Gly_{414}	Glu_{533}
Gly_{414}	Lys_{652}
Leu_{415}	Leu_{649}
Leu_{415}	Glu_{553}
Leu_{415}	Lys_{537}
Glu_{417}	Lys_{537}
Gly_{418}	Arg_{467}
Glu_{419}	Thr_{645}
Arg_{422}	Glu_{464}
Asp_{423}	Arg_{467}
Leu_{424}	Lys_{530}
Phe_{425}	Phe_{482}
Phe_{425}	Lys_{475}

In a second aspect, the present invention provides a method to identify an agent which modulates the interaction between pRb and $E2F_{(409\text{-}426)}$, the method comprising:-

a) combining together pRb, $E2F_{(409\text{-}426)}$ and an agent, under conditions in which pRb and $E2F_{(409\text{-}426)}$ form a complex;
b) growing a crystal of any pRb/$E2F_{(409\text{-}426)}$ complex; and
c) analysing the crystal structure to determine whether the agent is an agent which modulates the interaction between pRb and $E2F_{(409\text{-}426)}$.

In the present invention, the term "modulates" is intended to refer to inhibiting, enhancing, destabilising and/or stabilising the interaction between pRb and $E2F_{(409-426)}$ and/or the formation of the pRb/$E2F_{(409-426)}$ complex and/or the stability of the complex after formation.

"conditions in which pRb and $E2F_{(409-426)}$ can form a complex" are those conditions in which pRb and $E2F_{(409-426)}$ form a complex in the absence of an agent. Therefore the effect of the agent on the interaction between pRb and $E2F_{(409-426)}$ and complex formation can be assessed.

Growing a crystal of a pRb/$E2F_{(409-426)}$ complex in step b) can be performed using methods well known to the person skilled in the art, for example using methods described in Practical Protein Crystallography 1999, McRee, D. E., Academic Press, San Diego, Ca, USA; and also in Protein Crystallization Techniques, Strategies and Tips 1999, Bergfors, T. M., International University Line, Ca, USA.

In the method, the combining of the pRb, $E2F_{(409-426)}$ and agent may be in any order. The order may be combining pRb with the agent and then adding the $E2F_{(409-426)}$. Alternatively, the order may be combining $E2F_{(409-426)}$ with the agent and then adding pRb, or combining pRb with $E2F_{(409-426)}$ and then the agent. For example, the pRb may be combined with $E2F_{(409-426)}$ before soaking the complex in the agent, preferably in a solution of the agent. In this regard, two of the pRb, $E2F_{(409-426)}$ and agent may be co-crystalised before adding the pRb, $E2F_{(409-426)}$ or agent, as appropriate.

Preferably step c) comprises comparing the crystal structure to the crystal structure of the first aspect of the invention.

The agent may be selected using the three dimensional atomic co-ordinates of Annex 1.

In a third aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409\text{-}426)}$ complex, comprising selecting an agent using the three-dimensional atomic coordinates of Annex 1.

Preferably, said selection is performed in conjunction with computer modeling.

Preferably the method comprises the further steps of:

a) contacting the selected agent with pRb and E2F$_{(409\text{-}426)}$ under conditions in which pRb and E2F$_{(409\text{-}426)}$ can form a complex; and
b) measuring the binding affinity of pRb to E2F$_{(409\text{-}426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to E2F$_{(409\text{-}426)}$ when in the absence of the agent, wherein an agent modulates a pRb/E2F$_{(409\text{-}426)}$ complex when there is a change in the binding affinity of pRb to E2F$_{(409\text{-}426)}$ when in the presence of the agent.

The method may further comprise:

a) growing a supplementary crystal from a solution containing pRb and E2F$_{(409\text{-}426)}$ and the selected agent where said agent changes the binding affinity of the pRb/E2F$_{(409\text{-}426)}$ complex under conditions in which pRb and E2F$_{(409\text{-}426)}$ can form a complex;
b) determining the three-dimensional atomic co-ordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;
c) comparing the three dimensional atomic co-ordinates with those for the crystal structure as defined in the first aspect of the invention; and
d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal.

Preferably, said selection is performed in conjunction with computer modeling.

In a fourth aspect there is provided a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) contacting a selected agent with pRb and E2F$_{(409-426)}$ under conditions in which pRb and E2F$_{(409-426)}$ can form a complex; and
b) measuring the binding affinity of pRb to E2F$_{(409-426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to E2F$_{(409-426)}$ when in the absence of the agent, wherein an agent modulates a pRb/E2F$_{(409-426)}$ complex when there is a change in the binding affinity of pRb to E2F$_{(409-426)}$ when in the presence of the agent.

There is a "change in the binding affinity" when the binding affinity either decreases or increases when in the presence of the agent. If a decrease is observed, the agent may be inhibiting the complex. If an increase is observed, the agent may be enhancing the complex.

The method of the fourth aspect may further comprise:

a) growing a supplementary crystal from a solution containing pRb and E2F$_{(409-426)}$ and the selected agent where said agent changes the binding affinity of the pRb/E2F$_{(409-426)}$ complex under conditions in which pRb and E2F$_{(409-426)}$ can form a complex;
b) determining the three-dimensional atomic coordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;
c) comparing the three dimensional atomic co-ordinates with those for the crystal structure defined in the first aspect of the invention; and
d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal

Preferably, said selection is performed in conjunction with computer modeling.

In a fifth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb with the agent;
c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In a sixth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) crystalising pRb and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In a seventh aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb, E2F$_{(409-426)}$ and the agent;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

In an eighth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;

b) co-crystalising pRb and E2F$_{(409-426)}$ and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

Preferably the agent in the fifth, sixth, seventh or eighth aspect is selected using the three dimensional atomic co-ordinates of Annex 1. Preferably the method of the fifth, sixth, seventh or eighth aspect further comprises selecting a second generation agent using the three dimensional atomic coordinates determined. The second generation agent is preferably selected using the three dimensional atomic coordinates of Annex 1. The selection may be performed in conjunction with computer modeling.

Preferably the selected agent and/or the second generation agent, in the second, third, fourth, fifth, sixth, seventh and/or eighth aspects mimics a structural feature of E2F$_{(409-426)}$ when said E2F$_{(409-426)}$ is bound to pRb.

Preferably soaking refers to the pRb/E2F$_{(409-426)}$ complex being transferred to a solution containing the selected agent.

The method as defined in the third aspect preferably comprises the further steps of:
a) contacting the selected agent with a pRb/E2F$_{(409-426)}$ complex; and
b) determining whether the agent affects the stability of the complex.

Preferably the determination is with fluorescence polarization.

In a ninth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:
a) contacting a fluorescently tagged E2F$_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;

b) detecting the fluorescence polarization;

c) adding a selected agent; and

d) detecting the fluorescence polarization in the presence of the agent.

In a tenth aspect, the present invention provides a method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising;

a) contacting a fluorescently tagged E2F$_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;

b) detecting the fluorescence polarization;

c) contacting a selected agent with pRb and E2F$_{(409-426)}$ peptide (E2F-fluoropeptide) under conditions in which pRb and E2F-fluoropeptide can form a complex;

d) detecting the fluorescence polarization; and

e) comparing the fluorescence polarization detected in b) and d).

Preferably the fluorescently tagged E2F peptide is selected using the three dimensional atomic co-ordinates of Annex 1.

Preferably a decrease in fluorescence polarization in the presence of the agent indicates that the agent destabilises the complex.

The methods of the ninth or tenth aspects may comprise the further step of adding untagged E2F$_{(409-426)}$ and detecting fluorescence polarization.

Preferably if fluorescence polarization decreases , on addition of the untagged E2F$_{(409-426)}$, the agent does not stabilise the complex.

Preferably if there is no substantial change in fluorescence polarization, on addition of the untagged E2F$_{(409-426)}$, the agent stabilises the complex.

Preferably the method further comprises:

a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) adding an agent that modulates pRb/E2F$_{(409\text{-}426)}$ complex; and
d) detecting the fluorescence polarization in the presence of the agent.

Alternatively the method may further comprise:
a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) contacting an agent that modulates pRb/E2F$_{(409\text{-}426)}$ complex with pRb and E7-fluoropeptide under conditions in which pRb and E7-fluoropeptide can from a complex;
d) detecting the fluorescence polarization; and
e) comparing the fluorescence polarization detected in b) and d).

Preferably a decrease in fluorescence polarization indicates that the agent also inhibits E7 binding to pRb. Such agents can then be removed from the method because the agents are identified as non-specific inhibitors. This identification of non-specific inhibitors can dramatically reduce the workload downstream of the assay method, for example in biochemical assays, thereby accelerating the hit to lead discovery process.

In addition ANS (aniline naphthalene sulphonic acid) reagent may be used to detect hydrophobic surfaces on pRb which become exposed as it unfolds. The fluorescence of ANS is highly sensitive to its environment. In solution there is virtually no fluorescence, whereas when bound to protein, such as pRb, it fluoresces highly. Changes in protein structure can alter the fluorescent signal of bound ANS due to changes in its enviroment to water. Therefore changes in pRb structure can be detected on addition of ANS and the agent that modulates pRb/E2F$_{(409\text{-}426)}$ complex. If the fluorescent signal alters on addition of the agent, the agent may be affecting the pRb

structure. The use of ANS to monitor protein unfolding is known in the art (Semisotnov et al (1991) Biopolymers, 31(1), 119-128)

The binding affinities may be measured by isothermal titration calorimetry. Alternatively the binding affinities may be measured by Surface Plasmon Resonance (SPR).

In an eleventh aspect, the present invention provides an agent identified by a method according to the second, third, fourth, fifth, sixth, seventh, eighth, ninth and/or tenth aspects of the invention.

In a twelfth aspect, the present invention provides an agent, as set out according to the eleventh aspect of the invention, for use as an apoptosis promoting factor in the prevention or treatment of proliferative diseases.

Preferably the, or each selected agent is obtained from commercial sources or is synthesised. Preferably the agent is for use in preventing or treating cancer, which may be pancreatic cancer and related diseases.

In a thirteenth aspect, the present invention provides the use of an agent, which modulates a pRb/E2F$_{(409-426)}$ complex, identified by a method according to the second, third, fourth, fifth, sixth, seventh, eighth, ninth and/or tenth aspects of the present invention, in the manufacture of a medicament for the prevention or treatment of proliferative diseases.

The proliferative diseases may be cancer, preferably pancreatic cancer and related diseases.

In a fourteenth aspect, the present invention provides the use of the atomic co-ordinates of the crystal structure as set out according to the first aspect of the present invention, for identifying an agent that modulates a pRb/E2F$_{(409\text{-}426)}$ complex.

In a fifteenth aspect, the present invention provides computer readable media comprising a data storage material encoded with computer readable data, wherein said computer readable data comprises a set of atomic co-ordinates of the pRb/E2F$_{(409\text{-}426)}$ crystal structure according to Annex 1 recorded thereon.

Preferred features of each aspect of the invention are as for each of the other aspects *mutatis mutandis*.

The present invention will now be described, by way of example only, and with reference to the following figures, in which:

Annex I.

Atomic co-ordinates for crystal of pRb/E2F$_{(409\text{-}426)}$ complex.

In Annex 1 there is shown:

Column Number	*Description*
2	Atom number
3	Atom type
4	Residue type
5	pRb domains (A or B) or E2F$_{(409\text{-}426)}$ (P)
6	Residue number
7	x co-ordinate of atom (Å)
8	y co-ordinate of atom (Å)
9	z co-ordinate of atom (Å)
10	Occupancy
11	B-factor (Å^2)

Figure 1.

Structure of pRb/E2F.

(A) Schematic drawing of functional domains and protein constructs used for pRb, E2F. The shading used for the constructs in this panel match those used in subsequent figures.

(B) The structure of $pRb_{AB}/E2F_{(409-426)}$, shown in two orthogonal views in Ribbons representation. The helices of the A domain are shown as a darker shade to those of the B domain. The main-chain trace of E2F is labelled.

(C) The interactions between $E2F_{(409-426)}$ and pRb_{AB} are shown schematically with the E2F peptide running down the centre. Residues of E2F that are conserved across the five family members are shown as ovals, while the five residue subset of these conserved residues whose mutation leads to disruption of the pRb/E2F interaction are shaded. Hydrogen-bond interactions are shown as broken lines, while hydrophobic contacts are indicated by bands. Residues from domain A of pRb are labelled with an asterisk and the other residues are from domain B. All of the pRb residues shown are either invariant or conserved across 27 species of pRb, p107 and p130.

Figure 2.

Isothermal Titration Calorimetry (ITC) measurements.

(A) The upper panel shows the raw data of an ITC experiment performed at 22°C. The lower panel shows the integrated heat changes, corrected for the heat of dilution, and the fitted curve based on a single site model. The panel represents the experiment where $E2F_{(243-437)}$ is titrated into Rb_{AB}.

(B) Summary of dissociation constants obtained by ITC measurements. The quoted errors are those produced by fitting the data to a two-state model. For the interaction of $E2F_{(243-437)}$ to Rb_{AB} and Rb_{ABC} the affinities are too high to measure reliably and we have therefore quoted the upper limits of the dissociation constants.

Figure 3 – Binding of Fluorescein-E2F, Rhodamine-E2F and Fluorescein-E7 to pRb

Figure 4 – Displacement binding curves: **a)** $E2F_{409\text{-}426}$ peptide; **b)** detergent

Figure 5 – Screen controls from test screen 6 x 384 plates

Figure 6 – Correlation between inhibition of Rhodamine and Fluorescein-E2F

Figure 7 – Correlation between inhibition of Fluorescein-E2F and Fluorescein-E7

Figure 8 – **a)** Titration curves of rho-N-E2F (n=3); **b)** Time course of the change of fluorescence polarization signal with time taken from a test screen (mean±s.e.m., n=960)

Figure 9 – IC50 curves determined for hits identified using the screening protocol described with reference to Figures 3 to 8: **a)** hit compound IC50 curve; **b)** non-specific inhibitor IC50 curve

Structure determination of pRb/E2F

For crystallisation we used a pRb construct based on that previously described by Lee, J.O., Russo, A.A., and Pavletich, N.P. (1998). Structure of the retinoblastoma tumour-suppressor pocket domain bound to a peptide from HPV E7, Nature 391, 859-65, which has engineered thrombin cleavage sites at the ends of the flexible linker region between the A and B domains. Purification and proteolysis produces a final protein containing residues 372 to 589 of the A domain and 636 to 787 of the B domain (hereafter pRb_{AB} – Figure 1A). Although these two domains are not covalently attached after thrombin treatment, they remain tightly associated. The removal of the A-B linker region facilitates crystallisation of pRb but does not alter its binding affinity for E2F. Crystals of the $pRb/E2F_{(409\text{-}426)}$ complex grew in a plate-like

habit with typical dimensions 200 x 200 x 10 μm^3. Repeated attempts at data collection from flash-cooled crystals using synchrotron X-ray sources were thwarted by very high crystal mosaicity and poor data reduction statistics. The problem was overcome by using the micro-focus diffractometer on station ID13 at ESRF current experience and plans at EMBL and ESRF/ID13, Acta Crystallogr D 55, 1765-1770), currently the only such device installed at a synchrotron source. Using a 10x10 μm^2 aperture, data were collected from four separate and widely spaced volumes of a single crystal in order to minimise radiation damage. A total of 100, 1° oscillation images were collected using a MAR CCD detector. These data extended to a Bragg spacing of 2.5 Å with an overall R_{merge} = 9.2%, and completeness of 87%. The structure was solved by molecular replacement and produced initial electron density maps in which the E2F peptide ($E2F_{(409-426)}$) could be readily located.

Protein constructs.

Rb_{AB} was expressed as a GST-fusion protein in *E. coli* using the pGEX-6P vector. The construct was engineered to contain a Prescission protease site at the N-terminus of Rb as well as two thrombin sites (LVPRGS) inserted at either end of the flexible A-B linker. Fusion protein was loaded onto a glutathione Sepharose 4B column before treatment with thrombin and Prescission protease. The resulting eluent was further purified using a Superdex 200 gel filtration column. Rb_{ABC} was expressed in *E. coli* with a C-terminal His-tag using pET-24. Crude lysate was first purified using an S-sepharose column followed by a Ni-NTA step before being run on a Superdex 200 gel filtration column. Recombinant human $E2F1_{(243-437)}$ was expressed in *E. coli* using pGEX-6P with an engineered Prescission protease site at the N-terminus of E2F. Crude lysate was bound onto a glutathione Sepharose 4B column prior to cleavage with the protease. The resulting eluent was further purified by gel filtration on a Superdex 75 column. $E2F_{(409-426)}$ and $E2F_{(380-437)}$ were synthetic peptides. HPV-16 $E7_{(17-98)}$ was prepared as described elsewhere (Clements, A.J., K, Mazzareli, J.M. Ricciardi, R.P. Marmorstein R. (2000). Oligomerization properties of the viral

oncoproteins adenovirus E1A and human papillomavirus E7 and their complexes with the retinoblastoma protein., Biochemistry 39, 16033-16045).

Crystallography.

Plate-like crystals were grown by the hanging drop vapour diffusion method at 4°C. Rb_{AB} was mixed with the E2F-1 peptide at 1:2 molar ratio and concentrated to 15mg/ml. Hanging drops were formed by mixing 1μl of protein solution with an equal volume of reservoir solution containing; 0.14M Na citrate, 26% PEG400, 4% n-propanol and 0.1M Tris at pH 7.8. Crystals were flash frozen in mother-liquor made up to 25% glycerol. Diffraction data were collected using the micro-focus diffractometer at ESRF and processed using the DENZO and SCALEPACK software (Otwinowski, Z.M., W. (1993). In Data Collection and Processing, L.I. Sawyer, N. Bailey, S., ed. (SERC Daresbury Laboratory), pp. 556-562). Molecular replacement calculations were carried out using Amore (CCP4, 1994) with 1GUX.brk as the search model. The final model contains co-ordinates for the protein which cover residues 379-578 of the A domain and 644-787 of the B domain of Rb and the entire $E2F_{(409-426)}$ peptide for the four copies present in the asymmetric unit together with 600 solvent molecules. The refined model has the following residuals; R_{work} =23.7%, R_{free} =28.7%, rmsd bonds = 0.007 Å, rmsd angles =1.3°.

Structure of pRb/E2F complex

The packing of the A and B domains generates a waist-like interface groove into which $E2F_{(409-426)}$ binds in a largely extended manner (Figure 1B). The peptide makes contacts with residues from helices α4, α5, α6, α8 and α9 of domain A, and with α11 from domain B of pRb. Formation of the complex buries 2280 Å^2 of surface area, 1500 Å^2 of which are hydrophobic. The two end regions of the $E2F_{(409-426)}$ fragment make extensive contacts with pRb, while interactions made by the middle section of the $E2F_{(409-426)}$ fragment (residues 416 to 420) are relatively sparse (Figure 1C). Overall, a high proportion of the hydrogen bond interactions between the two

molecules involves the side chains of conserved pRb residues interacting with the main chain of E2F. Examination of the distribution of conserved residues over the surface of pRb, reveals that the majority are accounted for by the E2F binding site. There is a somewhat smaller cluster of conserved residues associated with the LxCxE binding site. Perhaps the most remarkable aspect of this analysis is that although pRb has been reported to associate with at least 110 cellular proteins perhaps 50 or more in a pocket-dependent manner, the E2F and LxCxE binding sites account for almost all of the conserved residues on its surface. There are two explanations that may partially account for these observations. Firstly, many of the reported binding partners of pRb have yet to be verified. Secondly, the LxCxE binding site is probably responsible for mediating the binding of many different proteins, such as HDAC, to pRb.

Since there are four copies of the pRb/E2F$_{(409-426)}$ complex in the asymmetric unit of our crystal form it is possible both to compare these four crystallographically independent copies of the pRb/E2F$_{(409-426)}$ complex and to compare them with the crystal structure of pRb/E7 without bond E2F (Lee et al., 1998 Supra). The first six residues at the N-terminus, the α3-α4 and α6-α7 loops adopt different conformations between the four copies in our asymmetric unit, while the variations across the rest of the structure between the four molecules is not significant. Comparison of the pRb structure in the presence and absence of bound E2F$_{(409-426)}$ shows that there is essentially no change in the relative orientation of the two lobes of the A/B pocket on E2F$_{(409-426)}$ binding nor any widespread changes in the structures of the individual domains. This comparison does reveal that the end of α4 and the connecting loop to α5 becomes ordered in the pRb/E2F$_{(409-426)}$ complex as two conserved residues (Glu464-pRb & Arg467-pRb located towards the end of α4 in our structure) interact with the E2F$_{(409-426)}$ peptide. Within the E2F$_{(409-426)}$ construct there are eight residues that are conserved across E2F's from all animal species (Figure 1A). Amino-acid substitutions at five of these positions have been shown to lead to loss of binding to pRb but retention of E2F's trans-activation potential. The following description

focuses on the structural role of these five residues. Tyr(411)-E2F appears to play an important role in peptide binding because its phenolic ring occupies a hydrophobic pocket created by Ile(536)-pRb, Ile(532)-pRb, Ile(547)-pRb and Phe(413)-E2F, while its hydroxyl group makes a hydrogen bond to the invariant Glu(554)-pRb. Towards the C-terminal part of the E2F peptide, Leu(424)-E2F and Phe(425)-E2F make several hydrophobic interactions, two of which involve conserved residues. Leu(424)-E2F makes contacts with the aliphatic portion of the side chain of Lys(530)-pRb and also packs against Leu(415)-E2F and Phe(425)-E2F. In addition, Phe(425)-E2F itself packs against Phe(482)-pRb. Unlike the residues of E2F just discussed, the side-chains of Glu(419)-E2F and Asp(423)-E2F do not point into the groove formed between the A and B domains of pRb, but instead point away from it. Glu(419)-E2F hydrogen bonds through a water molecule with the main-chain carbonyl of Thr(645)-pRb; Asp(423)-E2F forms a salt bridge with Arg(467)-pRb located at the end $\alpha 4$.

Finally, as described earlier, the crystal structure shows how E2F makes extensive contacts with largely conserved residues from both the A and B domains of the pocket and that the binding site for E2F is dependent on the structure of the interface between the two domains. This feature of the structure suggests that E2F acts as a sensor of the structural integrity of the pRb pocket. The position and nature of the E2F binding site make the binding of the transcription factor particularly sensitive to mutations in the pocket region of the tumour suppressor protein. The potential significance of these observations will be discussed later with regard to the normal role of pRb in protecting cells against E2F-mediated apoptosis.

Additional determinants of pRb/E2F function

It is clear from a number of studies that, although $E2F_{(409-426)}$ expressed as a Gal4 fusion protein is sufficient to recruit pRb and repress transcription, there are additional interactions made by the physiologically relevant E2F/DP heterodimer with pRb.

Similarly, while the pocket domain is highly conserved, the most frequent site of deleterious mutation, and capable of transcriptional repression, it is not sufficient for the physiological function of pRb. In particular, the C-terminus of pRb is necessary for mediating growth arrest and recruitment of certain cyclin/cdk complexes as well as containing several of the residues whose phosphorylation leads to deactivation of pRb function. Therefore, in order to better understand the requirements for physiological pRb/E2F complex formation, we have made a series of constructs of the two proteins (Figure 1A) and carried out binding measurements by isothermal titration calorimetry (ITC). We have also carried out a series of competition experiments to confirm qualitatively the interpretation of the ITC binding data.

Isothermal Titration Calorimetry.

Binding of the various E2F constructs to Rb_{AB} and Rb_{ABC} was measured by isothermal titration calorimetry using a MicroCal Omega VP-ITC machine (MicroCal Inc., Northampton, USA). The E2F constructs at a concentration between 100-150 μM were titrated into 12-15 μM Rb at a temperature of 22°C. Proteins were dialysed against 50mM Tris pH 7.6, 100mM NaCl and 1mM TCEP. After subtraction of the dilution heats, calorimetric data was analysed using the evaluation software MicroCal Origin v5.0 (MicroCal Software Inc.). For all of the titrations, the stoichiometry of ligand binding to Rb was very close to 1.0. For $E2F_{(243-437)}$ binding to Rb, the binding affinity and the heat change associated with binding were such that we could only establish that binding was tighter than 10 nM. In order to verify that binding of this protein was similar for both Rb_{AB} and Rb_{ABC} we carried out competition experiments which showed approximately equal partition between the two different Rb proteins.

Competition experiments.

The proteins used in these experiments were His_6-Rb_{ABC} (RESIDUES 380-929); MW 66.07kDa, non-tagged Rb_{AB} (residues 372-787); MW 48.67 KDa, are His_6-Rb_{AB} (residues 376-792); MW 49.86 KDa, $E2F_{(243-437)}$; MW 21.45 KDa HPV E7 (residues

17-98); MW 9.38 KDa and $E2F_{(409\text{-}426)}$; MW 2.12 KDa. Protein concentrations were carefully determined by u.v. spectroscopy and confirmed by ITC titrations. The small acidic E2F proteins stain much weaker than Rb with Coomassie on SDS-PAGE. For all gel lanes contained a final Rb_{AB} concentration of ca. 7μM. After equilibration with $E2F_{(243\text{-}437)}$ and $E2F_{(409\text{-}426)}$ the samples were loaded onto a 1.0ml Ni column and washed with 7 x 0.5 ml of loading buffer (50mM Tris pH 7.5, 200mM NaCl & 10mM Imidazole). The samples were then eluted with 7 x 0.5ml elution buffer (50mM Tris, pH 7.5, 200mM NaCl, 200mM Imidazole). After volume correction samples were boiled in SDS loading buffer and run on a 4-12% SDS PAGE. For the two pRb proteins and $E2F_{(243\text{-}437)}$ were mixed at 40μM in a final volume of 0.5ml. After equilibration for 2hrs the mixture was loaded onto 1ml Ni beads in a small column, washed with 7 x 0.5ml of loading buffer (50mM Tris, pH 7.5, 200mM NaCl, 10mM Imidazole), eluted using 7 x 0.5ml elution buffer (50mM Tris, pH 7.5, 200mM NaCl, 200mM Imidazole). Samples, after correcting for volume were boiled in SDS sample buffer and run on a 4-12% SDS gel.

A typical ITC experiment is shown in Figure 2A and a summary of the affinity constants obtained for both pRb_{AB} and pRb_{ABC} interacting with three constructs of E2F are given in Figure 2B. The two shorter E2F constructs bind to either pRb_{AB} or pRb_{ABC} with similar affinities. However, $E2F_{(243\text{-}437)}$ binds at least 16-fold stronger than either of the two shorter E2F fragments to both pRb_{AB} and Rb_{ABC}. Our ITC data therefore show that there are additional interactions of the A/B pocket of pRb with a region of E2F-1 outside of the transactivation domain. This result has been confirmed qualitatively by competition experiments which show that a 15-to 30-fold molar excess of the shorter E2F peptide is required to 50% compete with $E2F_{(243\text{-}437)}$ for binding to pRb. Our results are consistent with an earlier report that noted an interaction of pRb with the marked box region of E2F (residues 245-317). Taken together, these data demonstrate that the majority of the free energy of interaction between pRb and E2F is contributed by the 18-residue segment $E2F_{(409\text{-}426)}$ used in our

structure analysis. There is an additional stabilising interaction between the marked box region of E2F and pRb, that contributes approximately 2kcal mol^{-1} to the overall free energy of complex formation, but is not sufficient on its own for complex formation.

As the binding constant for the interaction of $E2F_{(243\text{-}437)}$ with pRb_{AB} (or pRb_{ABC}) was too tight to determine reliably by ITC we performed a competition experiment to determine if this E2F construct bound preferentially to one or the other pRb construct. The results show approximately equal partitioning of $E2F_{(243\text{-}437)}$ between the two pRb species and demonstrates therefore, that the C-terminus of pRb does not participate in the binding to E2F-1 in isolation. This means that in addition to the interaction of $E2F_{(409\text{-}426)}$ with the pocket region of pRb there is an additional interaction, almost certainly involving the marked box region of E2F, that also binds to the pRb pocket. This data is consistent with the hypothesis that the approximately 10-fold stronger interaction of E2F/DP with pRb_{ABC} rather than pRb_{AB} reported previously arises through interactions of the DP component of the E2F/DP heterodimer with the C-terminus of pRb. This idea is strongly supported by the data from another study which shows that DP-1 interacts with pRb in a manner that does not require the structural integrity of the A/B pocket. Taken together, these data indicate that at least one of the functions of the C-terminus of pRb is to bring additional stabilisation to the interaction of the tumour suppressor with the heterodimeric E2F/DP transcription factors.

Use of structure atomic co-ordinates of Annex I

The atomic co-ordinates of Annex 1 are cartesian co-ordinates derived from the results obtained on diffraction of a monochromatic beam of X-rays by the atoms of the pRb/ $E2F_{(409\text{-}26)}$ complex in crystal form. The diffraction data was used to calculate electron density maps of the crystal. The electron density maps were then used to position the individual atoms of the pRb/ $E2F_{(409\text{-}26)}$ complex.

The determination of the three-dimensional structure of the pRb/E2F$_{(409-426)}$ complex provides basis for the design of new and specific agents that modulates formation of the complex and/or modulates the interaction between pRb and E2F$_{(409-426)}$. For example, computer modelling programs may be used to design different molecules expected to modulate formation of the pRb/E2F$_{(409-426)}$ complex and/or the interactions between pRb and E2F$_{(409-426)}$.

A candidate agent, may be any available compound. A commercial library of compound structures such as the Cambridge Structural Database would enable computer based *in silico* screening of the databases to enable compounds that may interact with, and/or modulate formation of, the complex to be identified.

Such libraries may be used to allow computer-based high throughput screening of many compounds in order to identify and select those agents with potential to modulate formation of the pRb/E2F$_{(409-426)}$ complex and/or the interaction between pRb and E2F$_{(409-426)}$.

In this regard, a potential modulating agent can be subjected to computer modelling with a docking program such as GRAM, DOCK or AUTODOCK (see Walters et al., Drug discovery Today, Vol.3, No. 4, (1998), 160-178, and Dunbrack et al., Folding and Design, 2 (1997) 27-42) to identify and select potential agents. This can include computer fitting of potential modulating agents to the pRb/E2F$_{(409-426)}$ complex to ascertain how the agent, in terms of shape and structure, will bind to the complex.

Computer programs can be employed to estimate the interactions between the pRb, E2F$_{(409-426)}$ and agent or pRb/E2F$_{(409-426)}$ complex and agent. These interactions may be attraction, repulsion, and steric hindrance of the two binding partners (e.g. the pRb/E2F$_{(409-426)}$ complex and a selected agent). A potential agent will be expected to be more potent if there is a tighter fit and fewer steric hindrances, and therefore greater attractive forces.It is advantageous for the agent to be specific to reduce interaction

with other proteins. This could reduce the occurrence of side-effects due to additional interactions with other proteins.

Potential agents that have been designed or selected possible agents can then be screened for activity as set out in the second to tenth aspects above. The agents can be obtained from commercial sources or synthesised. The agent is then contacted with pRb/E2F$_{(409-426)}$ complex to determine the ability of the potential agent to modulate the formation of the complex. Alternatively the agent may be contacted with pRb and E2F$_{(409-426)}$ under conditions in which pRb and E2F$_{(409-426)}$ can form a complex (in the absence of agent), to determine the ability of the agent to modulate complex formation.

A complex of pRb/E2F$_{(409-426)}$ and said potential agent can then be formed such that the complex can be analysed by X-ray crystallography to determine the ability of the agent to modulate complex formation and/or the interaction between pRb and E2F$_{(409-426)}$.

The complex of pRb/E2F$_{(409-426)}$ and agent could be compared to that for pRb/E2F$_{(409-426)}$ alone with the three dimensional atomic co-ordinates in Annex 1.

Detailed structural information can then be obtained about the binding of the potential agent to the complex,. This will enable the structure or functionality of the potential agent to be altered to thereby to improve binding. The above steps may be repeated as may be required.

The agent-pRb/E2F$_{(409-426)}$ complex could be analysed by co-crystallising pRb/E2F$_{(409-426)}$ with the selected agent or soaking the agent into crystals of the pRb/E2F$_{(409-426)}$ complex; and then determining the three dimensional co-ordinates of the agent-complex by X-ray diffraction using molecular replacement analysis.

Therefore, the pRb/E2F$_{(409-426)}$ -agent complexes can be crystallised and analysed using X-ray diffraction data obtained and processed, for example using the DENZO and SCALEPACK software (Otwinowksi, Z. M., W. (1993). Difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallised pRb/E2F$_{(409-426)}$ complex and the solved structure of uncomplexed agent. These maps can then be used to determine the structure of the agent bound to the pRb/E2F$_{(409-426)}$ and/or changes in the conformation of pRb/E2F$_{(409-426)}$ complex relative to the pRb/E2F$_{(409-426)}$ complex in the absence of agent.

The agent may be improved, for example by adding or removing functional groups, substituting groups or altering its shape in light of data obtained from agent bound to pRb/E2F$_{(409-426)}$ complex and/or agent bound to pRb. Such an improved agent may then be subjected to the methods of the invention.

Electron density maps can be calculated using programs such Amore from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, Acta Crystallographical, D50, (1994), 760-763).

The provision of computer readable media enables the atomic co-ordinates to be accessed to model the pRb/E2F$_{(409-426)}$ complex by, for example, RAMSOL (a publicly available computer software package which allows access and analysis of atomic co-ordinate data for structure determination and/or rational drug design).

In addition, structure factor data, derivable from the atomic co-ordinate data (see e.g. Blundell et al., in Protein Crystallography, Academic Press, New York, London and San Francisco, (1976)), can be used to enable difference Fourier electron density maps to be deduced.

Screening assays

After an agent has been selected, its inhibitory effect on pRb/E2F$_{(409-426)}$ complex formation or ability to interact with the pRb/E2F$_{(409-426)}$ complex can be assessed with one or more of the methods of the invention.

For example, the crystal structure of the interaction of E2F$_{(409-426)}$ with pRb can be used to aid the design of a fluorescently tagged peptide for the use in a binding assay suitable for high throughput screening of low molecular weight compounds or peptide libraries. The fluorescent tag may be a fluorescein, rhodamine or some other commercially available tag chemically attached via a suitable amine or thiol group.

Binding could be measured by detecting fluorescence polarization in an homogeneous assay format (i.e. one in which all reagents are mixed in a single well, and reaction occurs in solution without wash steps). Fluorescence polarization technology is commonly applied in high throughput screening laboratories (ref: Sokham et al. (1999) Analytical Biochemistry, 275, 156-161. "Analysis of protein-peptide interaction by a miniaturised fluorescence polarization assay using cyclin-dependent kinase2/cyclin E as a model system.")

Fluorescence polarization can be used to determine binding of a fluorescently- tagged small molecule (ligand or peptide) with a large molecule (receptor or protein) by detecting changes in the rotational velocity of the small molecule in the free and bound state. The rotational velocity is inversely proportional to the size of the molecule. Using a fluorescently tagged peptide and suitable optics the changes in rotational velocity upon binding to pRb can be measured as a differences in light emitted in parallel and perpendicular to a polarized excitation source. Fluorescence polarisation gives a measure of the proportion of fluorescently tagged peptide found in the bound state in a homogenous format.

In an assay method of the present invention, fluoro-peptide (E2F$_{(409-426)}$ – fluoropeptide) bound to pRb will have a low rotational velocity and will appear

stationary during the excitation period. Emitted light will be transmitted in parallel to the polarized incident light and the light detected will have a high polarization value. In contrast in the presence of an inhibitor of the interaction between pRb and $E2F_{(409-426)}$-fluoropeptide, the free $E2F_{(409-426)}$- fluoro-peptide will have a high rotational velocity and light will be transmitted in all directions. Emitted light will be detected both parallel and perpendicular to the polarized excitation source, and will have a low polarization value.

An example of the use of fluorescence polarisation is now described.

Data from a Fluorescence Polarisation (FP) screen configured for the interaction of pRb with E2F is presented. Fluorescein-tagged E2F peptide was used to screen 10,000 small drug like molecules. Hit confirmation strategies based on fluorescence interference and specificity were developed and compared.

Based on the crystal structure defined by the atomic co-ordinates in Annex 1, an FP screen was configured for the interaction of recombinant pRb A/B domains with E2F(409-426) peptide (see Fig 1B). In addition, a second peptide binding site (E7, see Fig 1B), distant from the E2F binding pocket, was utilised as an internal control for non-specific inhibitors. Fluorophores in the form of fluorescein and rhodamine labelled peptides were synthesised and were used in a primary screen and hit confirmation.

Knowledge of the interaction of E2F and E7 peptides with pRb influenced the design of the fluoro-peptides used in the assay. The following peptides were synthesised, labelled and tested.

1. N-terminal amide linkage 5carboxyfluorescein-E2F409-426, 18'mer. (fl-N-E2F18)

LDYHFGLEEGEGIRDLFD

2. Rhodamine label at C-terminal cysteine E2F409-427, 19'mer. (Rh-C-E2F19)

LDYHFGLEEGEGIRDLFDC

3. Rhodamine label at DDC substitution E2F409-426, 18'mer. (Rh-N2-E2F18)

LCYHFGLEEGEGIRDLFD

4. N-terminal amide linkage 5carboxyfluorescein-E7, nonomer (Fl-E7)

DLYCYEQLN

Peptides 1, 3 and 4 were used in the screen and subsequent hit confirmation assays.

Synthetic peptides were synthesised and fluoro-tagged using either N-terminal labelling with 5 carboxyfluorescein succinimidyl ester or cysteine labelling with single isomer tetramethylrhodamine-5- maleimide. Typical titration binding curves of pRb with the fluoro-labelled peptides are shown (mean±sem, n=3) in Figure 3. Fluorescein fluorescence measured at λexcite = 485 and λemit = 520 nm
Rhodamine fluorescence measured at λexcite = 545 and λemit = 580 nm

Measurements were made using BMG Fluorostar plate reader fitted with polarization optic. Fluorescein-E2F showed the greatest degree of polarization, and consequently the best signal to noise. It was chosen as the label of choice for a primary screen. Data were fitted to a one site binding model using Graphpad prism. Kd values of

450± 70 and 380±50 nM were calculated for fluorescein and Rhodamine labelled E2F, which were similar to Kd determined for unlabelled peptide using isothermal calorimetry. Fluorescein-E7 showed tightest binding with Kd= 130±20 nM.

The assay principle was validated using unlabelled E2F peptide to displace Fl-E2F without disrupting Fl-E7 binding to pRb. Fluoro-tagged peptide (400 nM) was pre-incubated with pRb (1 μM) and unlabelled peptide added at the concentrations shown. Displacement binding curves were plotted (figure 4a), and were fitted to a one site competition binding model using Graphpad prism curve fitting software. These curves were compared to the effects of a detergent-like compound (figure 4b), which causes gross structural changes and disrupts binding of both peptides.

The results show that labelled E2F (Fl-E2F) does not displace E7, thereby validating the assay principle.

The assay was optimised in 384-well black plates (Matrix) and automated using a Beckman Fx liquid handling robot. 1 μM pRb in 50 mM Tris HCL, pH7.0, 100 mM NaCl, 10 mM DTT, 0.05% NP-40 was mixed with 40 μM compound (4% DMSO) and 0.4 μM fluorescein-E2F (final concentrations). Controls from a test screen of 10,000 compounds are shown in Figure 5.

Polarized and depolarized signal from fluorescein-E2F with and without pRb present are shown in Figure 5 (solid and open circles respectively). Specific disruption of binding by E2F protein and peptide are also shown. Addition of E2F protein completely displaces Fl-E2F (open triangle) and the signal is reduced to that of free fluoro-peptide alone. Addition of unlabelled-E2F at a concentration which gave 50% inhibition is clearly separated from the control populations. Hits were identified as compounds which reduced the polarization signal to less than mean-3sd of the fluorescein-E2F: pRb control.

Summary of Screen Data

Assay Principle		Fluorescence Polarization
Assay Automation		Biomek Fx
Assay Detection		BMG Polar Star Reader
Assay Parameters	Signal: noise	6.9
	Signal: background	4.8
	Z`	0.67
Test Screen 10,000	Z	0.45
	Hit rate	0.93%

Z factors are statistical factors well known by the skilled person in the art. The Z' factor is defined by

$$Z` = 1 - \left\{ \frac{(3X\ \mathbf{s.d.}\text{of positive control} + 3X\ \mathbf{s.d}\text{ of negative control})}{(\mathbf{mean}\text{ of positive control} - \mathbf{mean}\text{ of negative control})} \right\}$$

In the present assay:-

positive control = fully polarized signal; pRb plus fluoro-tagged E2F peptide

negative control = depolarized signal from fluoro-tagged E2F peptide alone.

Z is calculated in much the same way except:

Positive control = polarized signal of pRb and fluoro-tagged E2F in presence of compounds.

HIT CONFIRMATION:

Identification of Fluorescence Interfering Compounds.

A large proportion (37.5%) of the hits selected from the primary screen were coloured compounds which significantly altered the fluorescence intensity signal, and were potentially interfering with the assay. All hits were included in hit confirmation assays.

Hits were re-plated from master stocks and re-tested against fluorescein-E2F and rhodamine-E2F. A correlation (r^2=0.69) between inhibition of fluorescein E2F and Rhodamine-E2F was observed (figure 6) with a hit confirmation rate of 78%. Notably, 60% of compounds which were potentially interfering with the fluorescein signal were inhibitors with Rhodamine-E2F assay, without affecting rhodamine fluorescence intensity signal. Suggesting that deselection of compounds on the basis of fluorescence interference can lead to loss of real inhibitors.

Finally the hits were tested against a second peptide binding site. Fluorescein-E7 peptide at 400 nM. The results were compared to inhibition of E2F and a scatter plot is shown in Figure 7. A weak correlation was observed (r^2=0.51), with 72% of the inhibitors of E2F also inhibiting fluorescein E7. These compounds were excluded as non-specific inhibitors and were not taken forward in subsequent biochemical assays.

Comparison of Hit Confirmation Strategies on 80 best hits selected from a Primary screen of 10,000 compounds.

Hit Confirmation rates

Confirmation Test	% Primary Hits
1. Inhibition in retest Fluorescein-E2F	77.5
2. Fluorescence Interference	37.5
3. Inhibition in retest Rhodamine-E2F	62.5
4. Inhibition of Fluorescein-E7	58.5

The impact of selection strategy on number of compounds selected for further biochemical study (eg IC50, isothermal calorimetry, co-crystallisation)

Strategy 1	**Strategy 2**	**Strategy 3**
Tests 1+2 Remove fluorescence interfering compounds 36	Tests 1+3 Select inhibitors active for both fluorescein- and rhodamine-E2F 50	Tests 1+3+4 E2F inhibitors but not E7 inhibitors 14
False Negatives	False Positives	Specific Compounds only

To demonstrate the stability and rapidity of binding equilibria of fluoro-peptide with pRb. The titration curves shown in Figures 8a and 8b are typical of several experiments and are of rho-N-E2F (n=3). The time course shown of the change of fluorescence polarization signal with time is taken from a test screen (mean ± s.e.m., n= 960).

pRb titration curves were performed in 96-well black plates, in a total reaction volume of 100uL. Doubling dilutions from 10 μM stock of pRb were made in binding buffer (50 mM Tris HCL, pH7.0, 100 mM NaCl, 10 mM DTT, 0.05% NP-40) and 80 μL added in triplicate to wells. 20 μL of 2 μM fluoro-peptide was added and pipetted up and down to mix. The plate was read after 1 hr incubation at room temperature.

Compound interference was not a useful factor upon which to deselect compounds in an FP assay, and can lead to false negatives. The use of a second fluoro-label in hit confirmation avoids the loss of false negatives, but still includes false positives.

Screening of the hits against the second peptide site, E7, identified non-specific inhibitors, which caused gross structural changes to the protein. These were excluded from further biochemical testing. Identification of these non-specific inhibitors dramatically reduced the down stream work load.

The developed screening strategy rapidly identifies false negatives and positives (interfering and protein unfolding reagents) from the primary screen. This reduces the number of compounds to test in biochemical assays, thus saving both time and reagents which will accelerate the hit to lead discovery process.

ANS (aniline naphthalene sulphonic acid) reagent may be used to detect hydrophobic surfaces on pRb which become exposed as it unfolds. The fluorescence of ANS is highly sensitive to its environment. In solution there is virtually no fluorescence, whereas when bound to protein, such as pRb, it fluoresces highly. Changes in protein structure can alter the fluorescent signal of bound ANS due to changes in its environment to water. Therefore changes in pRb structure can be detected on addition of ANS and the agent that modulates pRb/E2F$_{(409-426)}$ complex. If the fluorescent signal alters on addition of the agent, the agent may be affecting the pRb structure. The use of ANS to monitor protein unfolding is known in the art (Semisotnov et al (1991) Biopolymers, 31(1), 119-128)

Biochemical assays could include IC50, isothermal calorimetry, and/or co-crystallisation.

In an example of an IC50 assay, reactions were performed in 96-well black plates in a total reaction volume of 100 µL. Compounds were dissolved in DMSO at a maximum concentration of 10 mM and doubling dilutions made in DMSO. 4 µL of diluted compound was mixed with 80 µL pRb (400 nM in binding buffer). The plate was incubated at room temperature for 15 min and then Rhodamine-E2F and fluorescein-

E7 were added to give final concentrations of 400 nM each. Reactions were performed in triplicate. Plates were read after 1 hr. The results are shown in Figures 9a and 9b.

Accordingly, an assay method could include the following steps:

a) allow complex formation of pRb and $E2F_{(409\text{-}426)}$-fluoropeptide, and measure maximum fluorescence polarization; and
b) add a selected agent and detect whether there is a decrease in fluorescence polarization.

Alternatively, an assay method could include the steps:

a) allow complex formation of pRb and $E2F_{(409\text{-}426)}$-fluoropeptide in the presence and absence of a selected agent and measure the fluorescence polarization; and
b) compare the fluorescence polarization values.

Compounds which stabilise the pRb/$E2F_{(409\text{-}426)}$ complex could be assessed in a modification of the above method, involving competition binding of pRb by unlabelled $E2F_{(409\text{-}426)}$ and $E2F_{(409\text{-}426)}$-fluoropeptide.

In this regard an assay method could include the following steps:

a) allow complex formation of pRb/$E2F_{(409\text{-}426)}$-fluoropeptide, and measure max fluorescence polarization;
b) add a selected agent and measure fluorescence polarization - if no change in fluorescence polarization there is no disruption of complex;
c) add unlabeled $E2F_{(409\text{-}426)}$ and measure fluorescence polarization - expect displacement of $E2F_{(409\text{-}426)}$-fluoropeptide and a decrease in fluorescence polarization, but not if complex is stabilised by presence of the agent.

Alternatively, the pRb, $E2F_{(409\text{-}426)}$-fluoropeptide and agent could be added together before detecting fluorescence polarization. If fluorescence polarization is reduced to

less than a predetermined value, the agent is determined to destabilize the complex, and vice versa.

The interactions could be confirmed by co-crystalisation of pRb/E2F$_{(409-426)}$ with the agent, and determination of the three dimensional atomic coordinates by X-ray diffraction and molecular replacement.

The E2F$_{(409-426)}$/pRb interaction can also be applied to heterogeneous assay formats (i.e. ones in which reagents are partitioned between a solid support and in solution, and wash steps are involved). This would involve the immobilisation of pRb on microtitre plates, for example by antibody capture or metal ion chelation using His-tagged pRb and Nickel coated plates. E2F$_{(409-426)}$ peptide may be tagged with fluorescence as above and the fluorescence detected directly to determine binding. Alternatively, the peptide could be labelled with biotin and detected with streptavidin-horse radish peroxidase in an ELISA-like format.

Compounds which interact with the complex without altering association or disassociation of the complex could be identified by crystallographic means, unless the agent itself was tagged (radioactivity/fluorescence) and binding to the complex measured directly, eg fluorescence polarization as above or scintallation counting of an immuno-precipitate.

Alternatively, the agent can be added to pRb and E2F$_{(409-26)}$ under conditions in which pRb and E2F$_{(409-26)}$ can form a complex. This could result in the agent and complex co-crystallising. The binding affinities of pRb to E2F$_{(409-26)}$ in the pRb/ E2F$_{(409-26)}$ complex in the presence and absence of the agent can then be compared to determine whether the agent inhibits complex formation. The three dimensional structure of the pRb/ E2F$_{(409-26)}$ – agent complex can also be solved (X-ray diffraction using molecular replacement analysis) to enable the associations in the new complex to be compared with those in the pRb/ E2F$_{(409-26)}$ complex (see Annex 1). As a further alternative the

pRb/ $E2F_{(409\text{-}26)}$ complex can be formed before soaking the complex in the presence of a selected agent. The binding affinities of pRb to $E2F_{(409\text{-}26)}$ can then be determined in the presence and absence of the agent. As before, the three dimensional structure of any pRb/ $E2F_{(409\text{-}26)}$ – agent complex could be solved.

The binding affinities can be measured using isothermal titration calorimetry. Alternatively, surface plasmon resonance (SPR) could be used such as that provided by Biacore AB.

Preferred features of each aspect of the invention are as for each of the other aspects *mutatis mutandis*. The prior art documents mentioned herein are incorporated to the fullest extent permitted by law.

Annex 1

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REMARK the coordinates is one molecule from four molecules in an asymmetric
REMARK unit cell whithin the crystal:
REMARK a=101.996  b=158.548  c=110.617  alpha=90.00  beta=93.70  gama=90.00 C 2
ATOM      1  N   MET A 379      13.261 -15.752  30.447  1.00 45.11           N
ATOM      2  CA  MET A 379      11.983 -16.486  30.626  1.00 44.12           C
ATOM      3  CB  MET A 379      11.935 -17.082  32.026  1.00 44.57           C
ATOM      4  CG  MET A 379      12.067 -16.066  33.137  1.00 45.87           C
ATOM      5  SD  MET A 379      12.458 -16.814  34.740  1.00 52.60           S
ATOM      6  CE  MET A 379      10.805 -17.831  35.114  1.00 52.37           C
ATOM      7  C   MET A 379      10.802 -15.543  30.446  1.00 43.32           C
ATOM      8  O   MET A 379       9.681 -15.889  30.824  1.00 43.69           O
ATOM      9  N   ASN A 380      11.069 -14.348  29.909  1.00 41.45           N
ATOM     10  CA  ASN A 380      10.043 -13.347  29.646  1.00 39.85           C
ATOM     11  CB  ASN A 380      10.641 -11.934  29.700  1.00 39.85           C
ATOM     12  CG  ASN A 380      10.867 -11.446  31.134  1.00 40.80           C
ATOM     13  OD1 ASN A 380       9.924 -11.442  31.937  1.00 40.97           O
ATOM     14  ND2 ASN A 380      12.115 -11.037  31.461  1.00 36.52           N
ATOM     15  C   ASN A 380       9.449 -13.550  28.273  1.00 38.62           C
ATOM     16  O   ASN A 380      10.144 -14.006  27.355  1.00 38.16           O
ATOM     17  N   THR A 381       8.174 -13.193  28.126  1.00 36.87           N
ATOM     18  CA  THR A 381       7.530 -13.259  26.812  1.00 35.53           C
ATOM     19  CB  THR A 381       6.303 -14.214  26.805  1.00 35.83           C
ATOM     20  OG1 THR A 381       5.350 -13.786  27.792  1.00 37.01           O
ATOM     21  CG2 THR A 381       6.717 -15.621  27.249  1.00 35.34           C
ATOM     22  C   THR A 381       7.123 -11.901  26.289  1.00 33.36           C
ATOM     23  O   THR A 381       6.745 -11.028  27.043  1.00 32.65           O
ATOM     24  N   ILE A 382       7.170 -11.770  24.971  1.00 31.97           N
ATOM     25  CA  ILE A 382       6.820 -10.549  24.266  1.00 30.21           C
ATOM     26  CB  ILE A 382       6.724 -10.881  22.782  1.00 30.35           C
ATOM     27  CG1 ILE A 382       6.672  -9.609  21.938  1.00 29.02           C
ATOM     28  CD1 ILE A 382       7.902  -8.721  22.081  1.00 33.06           C
ATOM     29  CG2 ILE A 382       5.534 -11.833  22.531  1.00 28.36           C
ATOM     30  C   ILE A 382       5.498 -10.020  24.767  1.00 29.89           C
ATOM     31  O   ILE A 382       5.258  -8.833  24.884  1.00 30.56           O
ATOM     32  N   GLN A 383       4.638 -10.942  25.092  1.00 29.58           N
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ATOM	33	CA	GLN	A	383	3.305	-10.639	25.574	1.00	29.76	C
ATOM	34	CB	GLN	A	383	2.535	-11.945	25.820	1.00	29.93	C
ATOM	35	CG	GLN	A	383	1.103	-11.705	26.237	1.00	34.71	C
ATOM	36	CD	GLN	A	383	0.261	-12.955	26.137	1.00	39.96	C
ATOM	37	OE1	GLN	A	383	-0.945	-12.917	26.383	1.00	39.55	O
ATOM	38	NE2	GLN	A	383	0.895	-14.071	25.754	1.00	43.51	N
ATOM	39	C	GLN	A	383	3.155	-9.723	26.795	1.00	27.99	C
ATOM	40	O	GLN	A	383	2.247	-8.901	26.822	1.00	27.26	O
ATOM	41	N	GLN	A	384	4.019	-9.868	27.792	1.00	26.56	N
ATOM	42	CA	GLN	A	384	3.915	-9.050	28.974	1.00	24.94	C
ATOM	43	CB	GLN	A	384	4.648	-9.689	30.147	1.00	26.49	C
ATOM	44	CG	GLN	A	384	6.156	-9.957	30.006	1.00	29.94	C
ATOM	45	CD	GLN	A	384	6.694	-10.838	31.188	1.00	35.67	C
ATOM	46	OE1	GLN	A	384	6.215	-11.970	31.425	1.00	33.73	O
ATOM	47	NE2	GLN	A	384	7.677	-10.306	31.921	1.00	37.23	N
ATOM	48	C	GLN	A	384	4.371	-7.617	28.771	1.00	23.54	C
ATOM	49	O	GLN	A	384	3.720	-6.670	29.241	1.00	23.14	O
ATOM	50	N	LEU	A	385	5.466	-7.419	28.053	1.00	21.30	N
ATOM	51	CA	LEU	A	385	5.894	-6.053	27.840	1.00	19.42	C
ATOM	52	CB	LEU	A	385	7.244	-5.976	27.128	1.00	20.05	C
ATOM	53	CG	LEU	A	385	7.786	-4.583	26.770	1.00	20.09	C
ATOM	54	CD1	LEU	A	385	7.807	-3.617	27.986	1.00	16.89	C
ATOM	55	CD2	LEU	A	385	9.205	-4.708	26.201	1.00	22.07	C
ATOM	56	C	LEU	A	385	4.848	-5.381	26.989	1.00	18.64	C
ATOM	57	O	LEU	A	385	4.598	-4.175	27.168	1.00	17.76	O
ATOM	58	N	MET	A	386	4.253	-6.140	26.050	1.00	16.78	N
ATOM	59	CA	MET	A	386	3.192	-5.561	25.195	1.00	16.27	C
ATOM	60	CB	MET	A	386	2.769	-6.488	24.033	1.00	16.13	C
ATOM	61	CG	MET	A	386	3.278	-6.115	22.679	1.00	14.44	C
ATOM	62	SD	MET	A	386	2.985	-7.361	21.343	1.00	20.61	S
ATOM	63	CE	MET	A	386	1.260	-6.895	20.591	1.00	17.31	C
ATOM	64	C	MET	A	386	1.953	-5.117	26.014	1.00	15.44	C
ATOM	65	O	MET	A	386	1.304	-4.152	25.688	1.00	14.45	O
ATOM	66	N	MET	A	387	1.641	-5.823	27.085	1.00	14.99	N
ATOM	67	CA	MET	A	387	0.500	-5.451	27.907	1.00	15.36	C
ATOM	68	CB	MET	A	387	0.080	-6.634	28.771	1.00	16.60	C
ATOM	69	CG	MET	A	387	-0.663	-7.709	28.039	1.00	21.28	C
ATOM	70	SD	MET	A	387	-1.472	-8.842	29.235	1.00	33.36	S

ATOM	71	CE	MET	A	387	-0.081	-9.970	29.834	1.00	29.39	C
ATOM	72	C	MET	A	387	0.815	-4.229	28.810	1.00	13.51	C
ATOM	73	O	MET	A	387	-0.019	-3.369	29.075	1.00	12.21	O
ATOM	74	N	ILE	A	388	2.043	-4.183	29.273	1.00	11.97	N
ATOM	75	CA	ILE	A	388	2.515	-3.099	30.071	1.00	10.08	C
ATOM	76	CB	ILE	A	388	3.933	-3.432	30.575	1.00	11.21	C
ATOM	77	CG1	ILE	A	388	3.834	-4.616	31.556	1.00	10.61	C
ATOM	78	CD1	ILE	A	388	5.163	-5.022	32.182	1.00	14.30	C
ATOM	79	CG2	ILE	A	388	4.646	-2.204	31.211	1.00	9.99	C
ATOM	80	C	ILE	A	388	2.484	-1.844	29.271	1.00	8.68	C
ATOM	81	O	ILE	A	388	1.938	-0.883	29.723	1.00	10.11	O
ATOM	82	N	LEU	A	389	3.028	-1.833	28.060	1.00	7.85	N
ATOM	83	CA	LEU	A	389	3.047	-0.600	27.248	1.00	6.29	C
ATOM	84	CB	LEU	A	389	4.037	-0.694	26.100	1.00	5.90	C
ATOM	85	CG	LEU	A	389	5.546	-0.953	26.392	1.00	5.99	C
ATOM	86	CD1	LEU	A	389	6.365	-0.770	25.087	1.00	2.00	C
ATOM	87	CD2	LEU	A	389	6.148	-0.133	27.549	1.00	4.06	C
ATOM	88	C	LEU	A	389	1.681	-0.189	26.740	1.00	6.09	C
ATOM	89	O	LEU	A	389	1.326	0.998	26.635	1.00	5.28	O
ATOM	90	N	ASN	A	390	0.872	-1.196	26.489	1.00	6.69	N
ATOM	91	CA	ASN	A	390	-0.485	-0.947	26.080	1.00	7.16	C
ATOM	92	CB	ASN	A	390	-1.197	-2.234	25.755	1.00	6.39	C
ATOM	93	CG	ASN	A	390	-1.054	-2.597	24.310	1.00	8.37	C
ATOM	94	OD1	ASN	A	390	-0.467	-1.844	23.505	1.00	7.04	O
ATOM	95	ND2	ASN	A	390	-1.582	-3.753	23.948	1.00	11.15	N
ATOM	96	C	ASN	A	390	-1.269	-0.146	27.084	1.00	7.15	C
ATOM	97	O	ASN	A	390	-2.038	0.694	26.653	1.00	9.07	O
ATOM	98	N	SER	A	391	-1.074	-0.344	28.385	1.00	6.14	N
ATOM	99	CA	SER	A	391	-1.849	0.461	29.338	1.00	7.59	C
ATOM	100	CB	SER	A	391	-2.517	-0.391	30.413	1.00	7.30	C
ATOM	101	OG	SER	A	391	-1.555	-1.006	31.241	1.00	6.73	O
ATOM	102	C	SER	A	391	-1.091	1.626	30.005	1.00	7.70	C
ATOM	103	O	SER	A	391	-1.696	2.512	30.608	1.00	6.83	O
ATOM	104	N	ALA	A	392	0.233	1.610	29.872	1.00	8.42	N
ATOM	105	CA	ALA	A	392	1.082	2.673	30.415	1.00	7.80	C
ATOM	106	CB	ALA	A	392	2.494	2.367	30.091	1.00	6.49	C
ATOM	107	C	ALA	A	392	0.695	4.043	29.860	1.00	8.43	C
ATOM	108	O	ALA	A	392	0.169	4.150	28.755	1.00	8.78	O

ATOM	109	N	SER	A	393	0.958	5.087	30.638	1.00	10.46	N
ATOM	110	CA	SER	A	393	0.655	6.482	30.310	1.00	11.12	C
ATOM	111	CB	SER	A	393	0.692	7.253	31.571	1.00	11.04	C
ATOM	112	OG	SER	A	393	0.415	8.586	31.290	1.00	15.76	O
ATOM	113	C	SER	A	393	1.651	7.157	29.385	1.00	12.00	C
ATOM	114	O	SER	A	393	2.838	6.842	29.408	1.00	13.27	O
ATOM	115	N	ASP	A	394	1.167	8.108	28.595	1.00	11.46	N
ATOM	116	CA	ASP	A	394	1.987	8.875	27.679	1.00	11.53	C
ATOM	117	CB	ASP	A	394	1.133	9.445	26.524	1.00	10.85	C
ATOM	118	CG	ASP	A	394	0.624	8.353	25.569	1.00	15.82	C
ATOM	119	OD1	ASP	A	394	1.378	7.926	24.658	1.00	17.94	O
ATOM	120	OD2	ASP	A	394	-0.509	7.835	25.673	1.00	18.22	O
ATOM	121	C	ASP	A	394	2.686	10.030	28.391	1.00	11.56	C
ATOM	122	O	ASP	A	394	3.497	10.760	27.796	1.00	12.74	O
ATOM	123	N	GLN	A	395	2.383	10.206	29.656	1.00	10.33	N
ATOM	124	CA	GLN	A	395	2.922	11.325	30.369	1.00	10.45	C
ATOM	125	CB	GLN	A	395	1.740	12.142	30.905	1.00	11.83	C
ATOM	126	CG	GLN	A	395	0.976	12.872	29.792	1.00	14.78	C
ATOM	127	CD	GLN	A	395	1.927	13.681	28.846	1.00	17.31	C
ATOM	128	OE1	GLN	A	395	1.612	13.884	27.668	1.00	13.52	O
ATOM	129	NE2	GLN	A	395	3.073	14.156	29.388	1.00	15.32	N
ATOM	130	C	GLN	A	395	3.822	10.878	31.519	1.00	8.54	C
ATOM	131	O	GLN	A	395	3.698	9.784	32.001	1.00	7.56	O
ATOM	132	N	PRO	A	396	4.735	11.724	31.946	1.00	7.59	N
ATOM	133	CA	PRO	A	396	5.567	11.391	33.102	1.00	8.16	C
ATOM	134	CB	PRO	A	396	6.401	12.675	33.324	1.00	6.76	C
ATOM	135	CG	PRO	A	396	6.360	13.350	32.081	1.00	6.09	C
ATOM	136	CD	PRO	A	396	5.063	13.040	31.373	1.00	6.71	C
ATOM	137	C	PRO	A	396	4.665	11.077	34.336	1.00	8.69	C
ATOM	138	O	PRO	A	396	3.600	11.699	34.508	1.00	9.77	O
ATOM	139	N	SER	A	397	5.084	10.162	35.184	1.00	8.42	N
ATOM	140	CA	SER	A	397	4.221	9.811	36.311	1.00	9.96	C
ATOM	141	CB	SER	A	397	4.561	8.437	36.910	1.00	9.22	C
ATOM	142	OG	SER	A	397	5.712	8.496	37.719	1.00	6.50	O
ATOM	143	C	SER	A	397	4.341	10.829	37.393	1.00	10.78	C
ATOM	144	O	SER	A	397	5.208	11.660	37.349	1.00	10.33	O
ATOM	145	N	GLU	A	398	3.475	10.725	38.380	1.00	12.24	N
ATOM	146	CA	GLU	A	398	3.529	11.583	39.523	1.00	15.01	C

ATOM	147	CB	GLU	A	398	2.442	11.150	40.497	1.00	16.05	C
ATOM	148	CG	GLU	A	398	1.144	10.725	39.763	1.00	22.93	C
ATOM	149	CD	GLU	A	398	0.312	11.914	39.223	1.00	30.62	C
ATOM	150	OE1	GLU	A	398	-0.005	12.877	40.018	1.00	28.54	O
ATOM	151	OE2	GLU	A	398	-0.016	11.876	37.984	1.00	34.64	O
ATOM	152	C	GLU	A	398	4.906	11.482	40.171	1.00	14.63	C
ATOM	153	O	GLU	A	398	5.503	12.440	40.559	1.00	14.38	O
ATOM	154	N	ASN	A	399	5.422	10.286	40.251	1.00	15.36	N
ATOM	155	CA	ASN	A	399	6.715	10.093	40.828	1.00	15.54	C
ATOM	156	CB	ASN	A	399	6.949	8.607	40.993	1.00	17.66	C
ATOM	157	CG	ASN	A	399	7.545	8.279	42.313	1.00	23.36	C
ATOM	158	OD1	ASN	A	399	8.739	8.543	42.555	1.00	29.18	O
ATOM	159	ND2	ASN	A	399	6.719	7.744	43.213	1.00	26.01	N
ATOM	160	C	ASN	A	399	7.843	10.673	40.001	1.00	14.48	C
ATOM	161	O	ASN	A	399	8.811	11.219	40.573	1.00	14.83	O
ATOM	162	N	LEU	A	400	7.747	10.584	38.663	1.00	11.35	N
ATOM	163	CA	LEU	A	400	8.829	11.137	37.861	1.00	9.12	C
ATOM	164	CB	LEU	A	400	8.722	10.696	36.425	1.00	8.94	C
ATOM	165	CG	LEU	A	400	9.965	10.282	35.637	1.00	7.91	C
ATOM	166	CD1	LEU	A	400	9.655	10.352	34.107	1.00	6.48	C
ATOM	167	CD2	LEU	A	400	11.217	11.040	35.988	1.00	6.99	C
ATOM	168	C	LEU	A	400	8.933	12.675	37.981	1.00	7.77	C
ATOM	169	O	LEU	A	400	10.029	13.239	38.047	1.00	7.08	O
ATOM	170	N	ILE	A	401	7.783	13.331	38.001	1.00	7.02	N
ATOM	171	CA	ILE	A	401	7.672	14.766	38.198	1.00	6.74	C
ATOM	172	CB	ILE	A	401	6.182	15.161	38.154	1.00	6.15	C
ATOM	173	CG1	ILE	A	401	5.669	15.045	36.732	1.00	7.60	C
ATOM	174	CD1	ILE	A	401	6.360	16.024	35.724	1.00	6.89	C
ATOM	175	CG2	ILE	A	401	5.968	16.588	38.665	1.00	4.00	C
ATOM	176	C	ILE	A	401	8.255	15.091	39.588	1.00	7.08	C
ATOM	177	O	ILE	A	401	8.872	16.141	39.834	1.00	6.41	O
ATOM	178	N	SER	A	402	8.112	14.141	40.479	1.00	6.89	N
ATOM	179	CA	SER	A	402	8.660	14.353	41.773	1.00	9.50	C
ATOM	180	CB	SER	A	402	8.347	13.166	42.680	1.00	10.22	C
ATOM	181	OG	SER	A	402	9.222	13.157	43.782	1.00	14.32	O
ATOM	182	C	SER	A	402	10.145	14.607	41.604	1.00	8.81	C
ATOM	183	O	SER	A	402	10.687	15.584	42.107	1.00	8.60	O
ATOM	184	N	TYR	A	403	10.799	13.744	40.852	1.00	9.20	N

ATOM	185	CA	TYR	A	403	12.231	13.941	40.585	1.00	9.67	C
ATOM	186	CB	TYR	A	403	12.780	12.753	39.816	1.00	9.50	C
ATOM	187	CG	TYR	A	403	13.035	11.498	40.641	1.00	10.54	C
ATOM	188	CD1	TYR	A	403	14.106	11.434	41.555	1.00	11.31	C
ATOM	189	CE1	TYR	A	403	14.355	10.307	42.276	1.00	9.55	C
ATOM	190	CZ	TYR	A	403	13.546	9.194	42.063	1.00	10.21	C
ATOM	191	OH	TYR	A	403	13.807	8.017	42.705	1.00	12.21	O
ATOM	192	CE2	TYR	A	403	12.514	9.224	41.171	1.00	6.97	C
ATOM	193	CD2	TYR	A	403	12.251	10.368	40.475	1.00	7.64	C
ATOM	194	C	TYR	A	403	12.579	15.264	39.824	1.00	9.18	C
ATOM	195	O	TYR	A	403	13.591	15.916	40.165	1.00	8.20	O
ATOM	196	N	PHE	A	404	11.751	15.634	38.836	1.00	7.17	N
ATOM	197	CA	PHE	A	404	11.953	16.876	38.133	1.00	8.77	C
ATOM	198	CB	PHE	A	404	10.904	17.114	36.997	1.00	9.18	C
ATOM	199	CG	PHE	A	404	10.887	16.043	35.902	1.00	6.14	C
ATOM	200	CD1	PHE	A	404	11.894	15.068	35.828	1.00	4.71	C
ATOM	201	CE1	PHE	A	404	11.866	14.087	34.869	1.00	2.70	C
ATOM	202	CZ	PHE	A	404	10.849	14.068	33.889	1.00	2.00	C
ATOM	203	CE2	PHE	A	404	9.856	15.048	33.939	1.00	2.00	C
ATOM	204	CD2	PHE	A	404	9.876	16.016	34.964	1.00	2.00	C
ATOM	205	C	PHE	A	404	11.909	18.081	39.104	1.00	10.04	C
ATOM	206	O	PHE	A	404	12.696	19.011	38.979	1.00	10.48	O
ATOM	207	N	ASN	A	405	10.991	18.073	40.060	1.00	10.29	N
ATOM	208	CA	ASN	A	405	10.927	19.164	41.005	1.00	11.87	C
ATOM	209	CB	ASN	A	405	9.546	19.150	41.687	1.00	13.31	C
ATOM	210	CG	ASN	A	405	8.446	19.650	40.757	1.00	14.99	C
ATOM	211	OD1	ASN	A	405	7.272	19.493	41.026	1.00	18.52	O
ATOM	212	ND2	ASN	A	405	8.844	20.265	39.670	1.00	12.65	N
ATOM	213	C	ASN	A	405	12.056	19.165	42.080	1.00	11.91	C
ATOM	214	O	ASN	A	405	12.255	20.149	42.813	1.00	10.19	O
ATOM	215	N	ASN	A	406	12.779	18.060	42.188	1.00	11.31	N
ATOM	216	CA	ASN	A	406	13.861	18.036	43.158	1.00	12.26	C
ATOM	217	CB	ASN	A	406	14.059	16.626	43.708	1.00	12.84	C
ATOM	218	CG	ASN	A	406	12.832	16.115	44.505	1.00	15.33	C
ATOM	219	OD1	ASN	A	406	12.327	16.823	45.337	1.00	18.94	O
ATOM	220	ND2	ASN	A	406	12.371	14.902	44.231	1.00	16.26	N
ATOM	221	C	ASN	A	406	15.190	18.520	42.617	1.00	12.01	C
ATOM	222	O	ASN	A	406	16.155	18.526	43.373	1.00	13.01	O

ATOM	223	N	CYS	A	407	15.245	18.845	41.316	1.00	10.65	N
ATOM	224	CA	CYS	A	407	16.454	19.284	40.629	1.00	9.58	C
ATOM	225	CB	CYS	A	407	16.358	19.051	39.114	1.00	9.61	C
ATOM	226	SG	CYS	A	407	16.101	17.366	38.388	1.00	7.04	S
ATOM	227	C	CYS	A	407	16.871	20.772	40.900	1.00	9.92	C
ATOM	228	O	CYS	A	407	16.056	21.660	41.100	1.00	10.76	O
ATOM	229	N	THR	A	408	18.163	21.036	40.929	1.00	9.20	N
ATOM	230	CA	THR	A	408	18.625	22.387	41.057	1.00	8.76	C
ATOM	231	CB	THR	A	408	20.132	22.403	40.955	1.00	9.46	C
ATOM	232	OG1	THR	A	408	20.746	21.698	42.061	1.00	10.38	O
ATOM	233	CG2	THR	A	408	20.691	23.859	41.004	1.00	8.49	C
ATOM	234	C	THR	A	408	18.050	23.190	39.890	1.00	8.65	C
ATOM	235	O	THR	A	408	17.807	24.356	40.027	1.00	9.13	O
ATOM	236	N	VAL	A	409	17.892	22.573	38.723	1.00	8.51	N
ATOM	237	CA	VAL	A	409	17.326	23.248	37.583	1.00	7.79	C
ATOM	238	CB	VAL	A	409	18.360	23.399	36.466	1.00	8.28	C
ATOM	239	CG1	VAL	A	409	17.817	24.215	35.268	1.00	6.45	C
ATOM	240	CG2	VAL	A	409	19.606	23.974	36.989	1.00	7.43	C
ATOM	241	C	VAL	A	409	16.213	22.344	37.104	1.00	8.17	C
ATOM	242	O	VAL	A	409	16.457	21.179	36.907	1.00	7.93	O
ATOM	243	N	ASN	A	410	15.007	22.876	36.914	1.00	7.49	N
ATOM	244	CA	ASN	A	410	13.864	22.062	36.530	1.00	8.42	C
ATOM	245	CB	ASN	A	410	12.566	22.786	36.929	1.00	8.29	C
ATOM	246	CG	ASN	A	410	11.361	21.860	36.935	1.00	7.78	C
ATOM	247	OD1	ASN	A	410	11.027	21.254	35.930	1.00	17.24	O
ATOM	248	ND2	ASN	A	410	10.706	21.767	38.037	1.00	2.36	N
ATOM	249	C	ASN	A	410	13.835	21.629	35.028	1.00	8.35	C
ATOM	250	O	ASN	A	410	13.852	22.453	34.141	1.00	7.62	O
ATOM	251	N	PRO	A	411	13.848	20.329	34.765	1.00	8.01	N
ATOM	252	CA	PRO	A	411	13.819	19.811	33.385	1.00	7.91	C
ATOM	253	CB	PRO	A	411	14.685	18.525	33.482	1.00	6.94	C
ATOM	254	CG	PRO	A	411	14.357	17.998	34.864	1.00	6.32	C
ATOM	255	CD	PRO	A	411	14.113	19.259	35.756	1.00	7.63	C
ATOM	256	C	PRO	A	411	12.470	19.497	32.786	1.00	8.05	C
ATOM	257	O	PRO	A	411	12.384	19.310	31.569	1.00	9.08	O
ATOM	258	N	LYS	A	412	11.422	19.458	33.581	1.00	8.49	N
ATOM	259	CA	LYS	A	412	10.086	19.154	33.046	1.00	9.75	C
ATOM	260	CB	LYS	A	412	9.052	19.504	34.066	1.00	9.19	C

ATOM	261	CG	LYS	A	412	7.744	18.856	33.805	1.00	12.96	C
ATOM	262	CD	LYS	A	412	6.730	19.221	34.859	1.00	20.30	C
ATOM	263	CE	LYS	A	412	5.921	20.478	34.478	1.00	22.28	C
ATOM	264	NZ	LYS	A	412	4.874	20.156	33.455	1.00	24.30	N
ATOM	265	C	LYS	A	412	9.717	19.867	31.717	1.00	10.16	C
ATOM	266	O	LYS	A	412	8.997	19.336	30.884	1.00	9.72	O
ATOM	267	N	GLU	A	413	10.253	21.055	31.526	1.00	10.93	N
ATOM	268	CA	GLU	A	413	9.971	21.858	30.354	1.00	12.98	C
ATOM	269	CB	GLU	A	413	10.335	23.314	30.655	1.00	14.77	C
ATOM	270	CG	GLU	A	413	9.876	24.252	29.569	1.00	22.12	C
ATOM	271	CD	GLU	A	413	8.366	24.221	29.395	1.00	30.57	C
ATOM	272	OE1	GLU	A	413	7.756	23.307	30.039	1.00	29.00	O
ATOM	273	OE2	GLU	A	413	7.827	25.111	28.609	1.00	33.99	O
ATOM	274	C	GLU	A	413	10.693	21.398	29.080	1.00	10.78	C
ATOM	275	O	GLU	A	413	10.082	21.129	28.015	1.00	10.26	O
ATOM	276	N	SER	A	414	12.000	21.334	29.166	1.00	8.08	N
ATOM	277	CA	SER	A	414	12.715	20.831	28.041	1.00	6.45	C
ATOM	278	CB	SER	A	414	14.174	20.915	28.308	1.00	5.87	C
ATOM	279	OG	SER	A	414	14.513	22.221	28.671	1.00	6.24	O
ATOM	280	C	SER	A	414	12.315	19.363	27.800	1.00	6.66	C
ATOM	281	O	SER	A	414	12.313	18.909	26.691	1.00	6.05	O
ATOM	282	N	ILE	A	415	11.998	18.602	28.836	1.00	7.08	N
ATOM	283	CA	ILE	A	415	11.537	17.282	28.494	1.00	9.05	C
ATOM	284	CB	ILE	A	415	11.925	16.069	29.384	1.00	8.83	C
ATOM	285	CG1	ILE	A	415	13.023	16.338	30.443	1.00	5.60	C
ATOM	286	CD1	ILE	A	415	13.107	15.477	31.689	1.00	2.00	C
ATOM	287	CG2	ILE	A	415	12.878	15.445	28.216	1.00	17.75	C
ATOM	288	C	ILE	A	415	10.274	17.026	27.672	1.00	8.74	C
ATOM	289	O	ILE	A	415	10.253	16.110	26.813	1.00	7.52	O
ATOM	290	N	LEU	A	416	9.241	17.788	27.974	1.00	7.71	N
ATOM	291	CA	LEU	A	416	8.015	17.661	27.301	1.00	7.92	C
ATOM	292	CB	LEU	A	416	6.969	18.514	28.017	1.00	7.90	C
ATOM	293	CG	LEU	A	416	6.634	18.055	29.452	1.00	11.36	C
ATOM	294	CD1	LEU	A	416	5.682	19.021	30.228	1.00	11.42	C
ATOM	295	CD2	LEU	A	416	6.048	16.647	29.484	1.00	3.28	C
ATOM	296	C	LEU	A	416	8.200	18.184	25.872	1.00	7.77	C
ATOM	297	O	LEU	A	416	7.621	17.588	24.900	1.00	8.01	O
ATOM	298	N	LYS	A	417	8.960	19.286	25.732	1.00	5.60	N

ATOM	299	CA	LYS	A	417	9.069	19.937	24.417	1.00	4.70	C
ATOM	300	CB	LYS	A	417	9.624	21.362	24.537	1.00	6.05	C
ATOM	301	CG	LYS	A	417	8.714	22.296	25.374	1.00	7.81	C
ATOM	302	CD	LYS	A	417	9.342	23.738	25.642	1.00	10.54	C
ATOM	303	CE	LYS	A	417	9.498	24.562	24.365	1.00	9.12	C
ATOM	304	NZ	LYS	A	417	8.200	24.843	23.770	1.00	5.02	N
ATOM	305	C	LYS	A	417	9.864	19.111	23.462	1.00	3.25	C
ATOM	306	O	LYS	A	417	9.522	18.992	22.249	1.00	2.53	O
ATOM	307	N	ARG	A	418	10.838	18.424	24.027	1.00	2.00	N
ATOM	308	CA	ARG	A	418	11.675	17.530	23.239	1.00	2.82	C
ATOM	309	CB	ARG	A	418	12.913	17.084	24.007	1.00	2.07	C
ATOM	310	CG	ARG	A	418	13.990	16.222	23.291	1.00	3.70	C
ATOM	311	CD	ARG	A	418	15.353	16.381	23.949	1.00	3.44	C
ATOM	312	NE	ARG	A	418	15.052	16.283	25.337	1.00	9.38	N
ATOM	313	CZ	ARG	A	418	15.626	16.901	26.313	1.00	6.00	C
ATOM	314	NH1	ARG	A	418	16.644	17.717	26.110	1.00	9.43	N
ATOM	315	NH2	ARG	A	418	15.149	16.666	27.520	1.00	7.51	N
ATOM	316	C	ARG	A	418	10.873	16.374	22.687	1.00	3.56	C
ATOM	317	O	ARG	A	418	11.026	16.045	21.472	1.00	3.39	O
ATOM	318	N	VAL	A	419	10.022	15.771	23.546	1.00	2.74	N
ATOM	319	CA	VAL	A	419	9.148	14.671	23.100	1.00	2.74	C
ATOM	320	CB	VAL	A	419	8.360	14.001	24.269	1.00	3.32	C
ATOM	321	CG1	VAL	A	419	7.306	13.052	23.758	1.00	2.00	C
ATOM	322	CG2	VAL	A	419	9.276	13.300	25.281	1.00	3.25	C
ATOM	323	C	VAL	A	419	8.193	15.168	21.994	1.00	2.42	C
ATOM	324	O	VAL	A	419	8.034	14.535	20.971	1.00	3.50	O
ATOM	325	N	LYS	A	420	7.615	16.337	22.159	1.00	3.84	N
ATOM	326	CA	LYS	A	420	6.751	16.936	21.135	1.00	6.62	C
ATOM	327	CB	LYS	A	420	6.277	18.304	21.639	1.00	9.19	C
ATOM	328	CG	LYS	A	420	4.764	18.548	21.803	1.00	12.82	C
ATOM	329	CD	LYS	A	420	4.215	19.176	20.530	1.00	18.36	C
ATOM	330	CE	LYS	A	420	4.359	18.239	19.264	1.00	22.97	C
ATOM	331	NZ	LYS	A	420	4.073	18.902	17.861	1.00	14.81	N
ATOM	332	C	LYS	A	420	7.452	17.114	19.771	1.00	6.45	C
ATOM	333	O	LYS	A	420	6.947	16.694	18.733	1.00	5.83	O
ATOM	334	N	ASP	A	421	8.638	17.722	19.772	1.00	7.00	N
ATOM	335	CA	ASP	A	421	9.337	17.999	18.503	1.00	5.93	C
ATOM	336	CB	ASP	A	421	10.454	19.038	18.683	1.00	5.34	C

ATOM	337	CG	ASP	A	421	9.935	20.397	19.244	1.00	10.31	C
ATOM	338	OD1	ASP	A	421	8.673	20.653	19.288	1.00	6.28	O
ATOM	339	OD2	ASP	A	421	10.768	21.259	19.696	1.00	14.34	O
ATOM	340	C	ASP	A	421	9.890	16.750	17.838	1.00	5.07	C
ATOM	341	O	ASP	A	421	9.683	16.527	16.652	1.00	6.86	O
ATOM	342	N	ILE	A	422	10.620	15.923	18.552	1.00	3.56	N
ATOM	343	CA	ILE	A	422	11.120	14.727	17.945	1.00	2.48	C
ATOM	344	CB	ILE	A	422	11.830	13.913	18.957	1.00	2.93	C
ATOM	345	CG1	ILE	A	422	13.031	14.638	19.545	1.00	2.54	C
ATOM	346	CD1	ILE	A	422	13.975	15.166	18.435	1.00	5.66	C
ATOM	347	CG2	ILE	A	422	12.172	12.511	18.367	1.00	2.78	C
ATOM	348	C	ILE	A	422	9.931	13.895	17.402	1.00	2.68	C
ATOM	349	O	ILE	A	422	9.990	13.371	16.355	1.00	2.00	O
ATOM	350	N	GLY	A	423	8.834	13.746	18.125	1.00	3.53	N
ATOM	351	CA	GLY	A	423	7.756	12.986	17.534	1.00	3.60	C
ATOM	352	C	GLY	A	423	7.330	13.576	16.190	1.00	5.15	C
ATOM	353	O	GLY	A	423	6.867	12.817	15.328	1.00	5.53	O
ATOM	354	N	TYR	A	424	7.468	14.901	16.007	1.00	3.70	N
ATOM	355	CA	TYR	A	424	6.999	15.558	14.812	1.00	4.56	C
ATOM	356	CB	TYR	A	424	6.996	17.095	14.956	1.00	4.66	C
ATOM	357	CG	TYR	A	424	6.643	17.772	13.661	1.00	2.59	C
ATOM	358	CD1	TYR	A	424	5.339	17.825	13.223	1.00	2.76	C
ATOM	359	CE1	TYR	A	424	5.024	18.381	12.022	1.00	3.68	C
ATOM	360	CZ	TYR	A	424	5.981	18.940	11.251	1.00	5.36	C
ATOM	361	OH	TYR	A	424	5.659	19.548	10.085	1.00	10.06	O
ATOM	362	CE2	TYR	A	424	7.274	18.940	11.653	1.00	6.09	C
ATOM	363	CD2	TYR	A	424	7.608	18.338	12.866	1.00	4.14	C
ATOM	364	C	TYR	A	424	7.946	15.174	13.665	1.00	4.75	C
ATOM	365	O	TYR	A	424	7.538	14.845	12.550	1.00	3.97	O
ATOM	366	N	ILE	A	425	9.208	15.194	13.996	1.00	5.11	N
ATOM	367	CA	ILE	A	425	10.246	14.814	13.086	1.00	6.31	C
ATOM	368	CB	ILE	A	425	11.575	15.256	13.706	1.00	7.12	C
ATOM	369	CG1	ILE	A	425	11.591	16.788	13.651	1.00	8.77	C
ATOM	370	CD1	ILE	A	425	12.912	17.423	13.998	1.00	11.84	C
ATOM	371	CG2	ILE	A	425	12.770	14.644	13.013	1.00	6.38	C
ATOM	372	C	ILE	A	425	10.245	13.338	12.694	1.00	6.08	C
ATOM	373	O	ILE	A	425	10.494	13.013	11.505	1.00	6.94	O
ATOM	374	N	PHE	A	426	9.942	12.475	13.661	1.00	4.61	N

ATOM	375	CA	PHE	A	426	9.951	11.028	13.521	1.00	4.17	C
ATOM	376	CB	PHE	A	426	9.753	10.393	14.915	1.00	3.43	C
ATOM	377	CG	PHE	A	426	9.726	8.882	14.904	1.00	4.06	C
ATOM	378	CD1	PHE	A	426	8.549	8.213	14.646	1.00	2.00	C
ATOM	379	CE1	PHE	A	426	8.518	6.847	14.597	1.00	2.00	C
ATOM	380	CZ	PHE	A	426	9.642	6.104	14.835	1.00	2.49	C
ATOM	381	CE2	PHE	A	426	10.861	6.767	15.101	1.00	5.74	C
ATOM	382	CD2	PHE	A	426	10.903	8.140	15.104	1.00	2.77	C
ATOM	383	C	PHE	A	426	8.872	10.489	12.555	1.00	5.54	C
ATOM	384	O	PHE	A	426	9.126	9.583	11.779	1.00	5.57	O
ATOM	385	N	LYS	A	427	7.651	11.011	12.633	1.00	6.97	N
ATOM	386	CA	LYS	A	427	6.582	10.546	11.739	1.00	7.52	C
ATOM	387	CB	LYS	A	427	5.192	11.052	12.102	1.00	7.33	C
ATOM	388	CG	LYS	A	427	4.705	10.664	13.535	1.00	13.06	C
ATOM	389	CD	LYS	A	427	3.495	11.526	13.935	1.00	21.22	C
ATOM	390	CE	LYS	A	427	3.309	11.580	15.408	1.00	28.07	C
ATOM	391	NZ	LYS	A	427	4.036	12.688	16.156	1.00	28.68	N
ATOM	392	C	LYS	A	427	6.880	10.870	10.317	1.00	5.90	C
ATOM	393	O	LYS	A	427	6.715	10.025	9.441	1.00	6.60	O
ATOM	394	N	GLU	A	428	7.364	12.069	10.081	1.00	5.34	N
ATOM	395	CA	GLU	A	428	7.608	12.462	8.709	1.00	5.59	C
ATOM	396	CB	GLU	A	428	7.930	13.958	8.614	1.00	5.72	C
ATOM	397	CG	GLU	A	428	6.890	14.894	9.187	1.00	6.84	C
ATOM	398	CD	GLU	A	428	5.572	14.861	8.439	1.00	12.45	C
ATOM	399	OE1	GLU	A	428	5.630	14.955	7.186	1.00	19.41	O
ATOM	400	OE2	GLU	A	428	4.475	14.734	9.075	1.00	8.62	O
ATOM	401	C	GLU	A	428	8.720	11.563	8.091	1.00	4.41	C
ATOM	402	O	GLU	A	428	8.634	11.081	6.969	1.00	3.48	O
ATOM	403	N	LYS	A	429	9.745	11.339	8.883	1.00	4.31	N
ATOM	404	CA	LYS	A	429	10.831	10.497	8.509	1.00	4.32	C
ATOM	405	CB	LYS	A	429	11.939	10.610	9.514	1.00	4.54	C
ATOM	406	CG	LYS	A	429	12.655	11.990	9.432	1.00	5.96	C
ATOM	407	CD	LYS	A	429	14.004	12.046	10.143	1.00	5.92	C
ATOM	408	CE	LYS	A	429	14.709	13.432	9.940	1.00	5.19	C
ATOM	409	NZ	LYS	A	429	16.072	13.456	10.579	1.00	3.04	N
ATOM	410	C	LYS	A	429	10.404	9.085	8.301	1.00	4.70	C
ATOM	411	O	LYS	A	429	10.740	8.458	7.295	1.00	3.93	O
ATOM	412	N	PHE	A	430	9.557	8.607	9.197	1.00	6.56	N

ATOM	413	CA	PHE	A	430	9.124	7.229	9.124	1.00	7.38	C
ATOM	414	CB	PHE	A	430	8.236	6.911	10.323	1.00	7.54	C
ATOM	415	CG	PHE	A	430	7.907	5.450	10.464	1.00	8.61	C
ATOM	416	CD1	PHE	A	430	7.066	4.830	9.564	1.00	11.42	C
ATOM	417	CE1	PHE	A	430	6.769	3.531	9.687	1.00	12.86	C
ATOM	418	CZ	PHE	A	430	7.329	2.825	10.689	1.00	13.90	C
ATOM	419	CE2	PHE	A	430	8.207	3.404	11.558	1.00	9.63	C
ATOM	420	CD2	PHE	A	430	8.469	4.699	11.469	1.00	7.48	C
ATOM	421	C	PHE	A	430	8.411	7.061	7.772	1.00	7.72	C
ATOM	422	O	PHE	A	430	8.846	6.303	6.897	1.00	6.61	O
ATOM	423	N	ALA	A	431	7.334	7.807	7.602	1.00	8.28	N
ATOM	424	CA	ALA	A	431	6.583	7.787	6.355	1.00	10.41	C
ATOM	425	CB	ALA	A	431	5.660	8.974	6.307	1.00	9.96	C
ATOM	426	C	ALA	A	431	7.482	7.834	5.109	1.00	13.02	C
ATOM	427	O	ALA	A	431	7.248	7.119	4.125	1.00	11.76	O
ATOM	428	N	LYS	A	432	8.494	8.710	5.142	1.00	15.88	N
ATOM	429	CA	LYS	A	432	9.407	8.866	4.022	1.00	18.85	C
ATOM	430	CB	LYS	A	432	10.328	10.025	4.327	1.00	20.32	C
ATOM	431	CG	LYS	A	432	11.123	10.540	3.144	1.00	25.80	C
ATOM	432	CD	LYS	A	432	12.118	11.692	3.537	1.00	32.56	C
ATOM	433	CE	LYS	A	432	11.389	12.923	4.109	1.00	36.99	C
ATOM	434	NZ	LYS	A	432	12.281	14.009	4.701	1.00	35.79	N
ATOM	435	C	LYS	A	432	10.218	7.574	3.842	1.00	19.52	C
ATOM	436	O	LYS	A	432	10.266	7.003	2.783	1.00	19.79	O
ATOM	437	N	ALA	A	433	10.789	7.038	4.909	1.00	20.45	N
ATOM	438	CA	ALA	A	433	11.573	5.818	4.747	1.00	20.25	C
ATOM	439	CB	ALA	A	433	12.205	5.439	6.008	1.00	19.25	C
ATOM	440	C	ALA	A	433	10.685	4.696	4.273	1.00	20.97	C
ATOM	441	O	ALA	A	433	11.085	3.860	3.522	1.00	19.77	O
ATOM	442	N	VAL	A	434	9.471	4.656	4.772	1.00	23.20	N
ATOM	443	CA	VAL	A	434	8.589	3.571	4.450	1.00	24.82	C
ATOM	444	CB	VAL	A	434	7.473	3.514	5.426	1.00	23.74	C
ATOM	445	CG1	VAL	A	434	6.429	2.537	4.929	1.00	26.52	C
ATOM	446	CG2	VAL	A	434	7.992	3.073	6.705	1.00	26.22	C
ATOM	447	C	VAL	A	434	8.011	3.810	3.087	1.00	26.57	C
ATOM	448	O	VAL	A	434	7.026	4.512	2.937	1.00	28.03	O
ATOM	449	N	GLY	A	435	8.605	3.225	2.071	1.00	28.57	N
ATOM	450	CA	GLY	A	435	8.073	3.426	0.753	1.00	30.76	C

ATOM	451	C	GLY	A	435	7.687	4.898	0.666	1.00	32.32	C
ATOM	452	O	GLY	A	435	8.546	5.752	0.859	1.00	32.41	O
ATOM	453	N	GLN	A	436	6.401	5.184	0.440	1.00	32.95	N
ATOM	454	CA	GLN	A	436	5.958	6.530	0.236	1.00	34.18	C
ATOM	455	CB	GLN	A	436	6.058	6.779	-1.265	1.00	35.09	C
ATOM	456	CG	GLN	A	436	7.501	6.823	-1.799	1.00	38.55	C
ATOM	457	CD	GLN	A	436	7.698	6.064	-3.115	1.00	40.82	C
ATOM	458	OE1	GLN	A	436	8.670	6.317	-3.836	1.00	42.49	O
ATOM	459	NE2	GLN	A	436	6.778	5.145	-3.431	1.00	41.77	N
ATOM	460	C	GLN	A	436	4.522	6.874	0.738	1.00	34.26	C
ATOM	461	O	GLN	A	436	3.675	5.955	0.911	1.00	34.87	O
ATOM	462	N	GLY	A	437	4.278	8.185	0.952	1.00	32.88	N
ATOM	463	CA	GLY	A	437	2.979	8.731	1.293	1.00	32.07	C
ATOM	464	C	GLY	A	437	2.649	9.129	2.729	1.00	31.84	C
ATOM	465	O	GLY	A	437	3.329	9.947	3.330	1.00	33.28	O
ATOM	466	N	CYS	A	438	1.569	8.559	3.264	1.00	30.09	N
ATOM	467	CA	CYS	A	438	1.081	8.811	4.618	1.00	28.02	C
ATOM	468	CB	CYS	A	438	-0.349	9.405	4.591	1.00	28.75	C
ATOM	469	SG	CYS	A	438	-1.524	8.660	5.796	1.00	30.36	S
ATOM	470	C	CYS	A	438	1.019	7.448	5.270	1.00	26.25	C
ATOM	471	O	CYS	A	438	0.383	6.535	4.724	1.00	24.75	O
ATOM	472	N	VAL	A	439	1.680	7.320	6.426	1.00	24.37	N
ATOM	473	CA	VAL	A	439	1.801	6.035	7.132	1.00	22.64	C
ATOM	474	CB	VAL	A	439	3.252	5.510	7.079	1.00	22.72	C
ATOM	475	CG1	VAL	A	439	3.330	4.007	7.496	1.00	22.50	C
ATOM	476	CG2	VAL	A	439	3.826	5.722	5.695	1.00	22.13	C
ATOM	477	C	VAL	A	439	1.303	6.064	8.591	1.00	21.76	C
ATOM	478	O	VAL	A	439	2.080	6.166	9.531	1.00	18.79	O
ATOM	479	N	GLU	A	440	-0.016	5.952	8.749	1.00	21.55	N
ATOM	480	CA	GLU	A	440	-0.623	5.986	10.061	1.00	21.30	C
ATOM	481	CB	GLU	A	440	-2.104	5.639	9.974	1.00	22.04	C
ATOM	482	CG	GLU	A	440	-2.941	6.602	9.153	1.00	23.35	C
ATOM	483	CD	GLU	A	440	-4.398	6.142	9.025	1.00	27.57	C
ATOM	484	OE1	GLU	A	440	-4.964	5.665	10.046	1.00	29.99	O
ATOM	485	OE2	GLU	A	440	-5.002	6.237	7.914	1.00	27.95	O
ATOM	486	C	GLU	A	440	0.081	5.115	11.119	1.00	20.38	C
ATOM	487	O	GLU	A	440	-0.247	5.193	12.283	1.00	21.06	O
ATOM	488	N	ILE	A	441	1.098	4.348	10.760	1.00	19.36	N

ATOM	489	CA	ILE	A	441	1.691	3.450	11.758	1.00	18.24	C
ATOM	490	CB	ILE	A	441	2.085	2.105	11.088	1.00	18.75	C
ATOM	491	CG1	ILE	A	441	0.893	1.146	11.125	1.00	21.67	C
ATOM	492	CD1	ILE	A	441	-0.283	1.567	10.160	1.00	26.94	C
ATOM	493	CG2	ILE	A	441	3.147	1.404	11.844	1.00	22.00	C
ATOM	494	C	ILE	A	441	2.832	4.072	12.555	1.00	16.39	C
ATOM	495	O	ILE	A	441	3.166	3.652	13.665	1.00	15.75	O
ATOM	496	N	GLY	A	442	3.440	5.089	11.968	1.00	14.93	N
ATOM	497	CA	GLY	A	442	4.514	5.798	12.581	1.00	13.46	C
ATOM	498	C	GLY	A	442	4.109	6.399	13.897	1.00	14.00	C
ATOM	499	O	GLY	A	442	4.862	6.323	14.833	1.00	16.06	O
ATOM	500	N	SER	A	443	2.940	7.002	13.990	1.00	13.14	N
ATOM	501	CA	SER	A	443	2.463	7.538	15.243	1.00	12.84	C
ATOM	502	CB	SER	A	443	1.049	8.104	15.060	1.00	12.90	C
ATOM	503	OG	SER	A	443	1.074	9.243	14.212	1.00	17.50	O
ATOM	504	C	SER	A	443	2.366	6.520	16.346	1.00	12.40	C
ATOM	505	O	SER	A	443	2.867	6.744	17.417	1.00	12.76	O
ATOM	506	N	GLN	A	444	1.694	5.409	16.075	1.00	12.47	N
ATOM	507	CA	GLN	A	444	1.407	4.381	17.069	1.00	12.70	C
ATOM	508	CB	GLN	A	444	0.527	3.245	16.467	1.00	12.40	C
ATOM	509	CG	GLN	A	444	0.280	1.987	17.407	1.00	17.53	C
ATOM	510	CD	GLN	A	444	-1.153	1.909	18.097	1.00	20.42	C
ATOM	511	OE1	GLN	A	444	-1.419	2.577	19.145	1.00	19.65	O
ATOM	512	NE2	GLN	A	444	-2.048	1.106	17.506	1.00	16.04	N
ATOM	513	C	GLN	A	444	2.729	3.893	17.660	1.00	11.87	C
ATOM	514	O	GLN	A	444	2.833	3.634	18.875	1.00	10.62	O
ATOM	515	N	ARG	A	445	3.765	3.836	16.821	1.00	10.93	N
ATOM	516	CA	ARG	A	445	5.022	3.341	17.337	1.00	10.57	C
ATOM	517	CB	ARG	A	445	5.910	2.901	16.201	1.00	12.33	C
ATOM	518	CG	ARG	A	445	5.318	1.798	15.401	1.00	15.05	C
ATOM	519	CD	ARG	A	445	6.277	1.028	14.668	1.00	20.23	C
ATOM	520	NE	ARG	A	445	5.592	0.089	13.790	1.00	27.54	N
ATOM	521	CZ	ARG	A	445	6.170	-0.577	12.776	1.00	29.64	C
ATOM	522	NH1	ARG	A	445	7.471	-0.444	12.508	1.00	26.97	N
ATOM	523	NH2	ARG	A	445	5.432	-1.411	12.047	1.00	32.65	N
ATOM	524	C	ARG	A	445	5.751	4.342	18.236	1.00	9.95	C
ATOM	525	O	ARG	A	445	6.220	3.973	19.354	1.00	9.16	O
ATOM	526	N	TYR	A	446	5.860	5.593	17.764	1.00	7.68	N

ATOM	527	CA	TYR	A	446	6.505	6.634	18.558	1.00	6.37	C
ATOM	528	CB	TYR	A	446	6.448	7.988	17.835	1.00	6.60	C
ATOM	529	CG	TYR	A	446	7.190	9.082	18.575	1.00	3.78	C
ATOM	530	CD1	TYR	A	446	8.564	9.103	18.559	1.00	2.15	C
ATOM	531	CE1	TYR	A	446	9.264	10.019	19.243	1.00	2.00	C
ATOM	532	CZ	TYR	A	446	8.646	10.974	19.966	1.00	2.00	C
ATOM	533	OH	TYR	A	446	9.472	11.916	20.558	1.00	2.42	O
ATOM	534	CE2	TYR	A	446	7.293	11.020	20.022	1.00	2.00	C
ATOM	535	CD2	TYR	A	446	6.533	10.064	19.311	1.00	2.00	C
ATOM	536	C	TYR	A	446	5.895	6.730	19.983	1.00	5.32	C
ATOM	537	O	TYR	A	446	6.611	6.820	20.978	1.00	3.64	O
ATOM	538	N	LYS	A	447	4.568	6.669	20.054	1.00	3.91	N
ATOM	539	CA	LYS	A	447	3.856	6.656	21.333	1.00	3.14	C
ATOM	540	CB	LYS	A	447	2.336	6.580	21.139	1.00	2.11	C
ATOM	541	CG	LYS	A	447	1.767	7.958	20.756	1.00	4.83	C
ATOM	542	CD	LYS	A	447	0.326	7.986	20.456	1.00	12.30	C
ATOM	543	CE	LYS	A	447	-0.122	9.423	19.935	1.00	19.61	C
ATOM	544	NZ	LYS	A	447	0.615	9.946	18.721	1.00	25.13	N
ATOM	545	C	LYS	A	447	4.301	5.563	22.287	1.00	3.08	C
ATOM	546	O	LYS	A	447	4.442	5.807	23.476	1.00	2.00	O
ATOM	547	N	LEU	A	448	4.487	4.354	21.742	1.00	3.95	N
ATOM	548	CA	LEU	A	448	4.899	3.219	22.509	1.00	3.91	C
ATOM	549	CB	LEU	A	448	4.829	1.917	21.677	1.00	4.54	C
ATOM	550	CG	LEU	A	448	3.444	1.290	21.488	1.00	6.42	C
ATOM	551	CD1	LEU	A	448	3.498	0.126	20.480	1.00	4.90	C
ATOM	552	CD2	LEU	A	448	2.885	0.833	22.829	1.00	2.56	C
ATOM	553	C	LEU	A	448	6.327	3.501	22.949	1.00	3.00	C
ATOM	554	O	LEU	A	448	6.724	3.194	24.097	1.00	2.00	O
ATOM	555	N	GLY	A	449	7.089	4.088	22.029	1.00	2.24	N
ATOM	556	CA	GLY	A	449	8.440	4.523	22.383	1.00	3.49	C
ATOM	557	C	GLY	A	449	8.432	5.426	23.628	1.00	4.47	C
ATOM	558	O	GLY	A	449	9.127	5.100	24.600	1.00	5.55	O
ATOM	559	N	VAL	A	450	7.586	6.473	23.665	1.00	3.49	N
ATOM	560	CA	VAL	A	450	7.575	7.363	24.792	1.00	4.55	C
ATOM	561	CB	VAL	A	450	6.399	8.319	24.875	1.00	6.58	C
ATOM	562	CG1	VAL	A	450	6.709	9.670	25.552	1.00	7.93	C
ATOM	563	CG2	VAL	A	450	5.813	8.538	23.636	1.00	13.08	C
ATOM	564	C	VAL	A	450	7.157	6.676	26.043	1.00	3.61	C

ATOM	565	O	VAL	A	450	7.611	7.058	27.139	1.00	2.67	O
ATOM	566	N	ARG	A	451	6.181	5.784	25.926	1.00	2.00	N
ATOM	567	CA	ARG	A	451	5.688	5.160	27.117	1.00	2.00	C
ATOM	568	CB	ARG	A	451	4.415	4.350	26.864	1.00	2.00	C
ATOM	569	CG	ARG	A	451	3.265	5.172	26.369	1.00	2.00	C
ATOM	570	CD	ARG	A	451	2.114	4.324	25.965	1.00	5.40	C
ATOM	571	NE	ARG	A	451	0.956	5.069	25.455	1.00	10.15	N
ATOM	572	CZ	ARG	A	451	-0.248	4.474	25.274	1.00	14.62	C
ATOM	573	NH1	ARG	A	451	-0.364	3.167	25.570	1.00	13.39	N
ATOM	574	NH2	ARG	A	451	-1.326	5.159	24.828	1.00	11.66	N
ATOM	575	C	ARG	A	451	6.801	4.316	27.772	1.00	2.00	C
ATOM	576	O	ARG	A	451	6.862	4.221	28.985	1.00	2.06	O
ATOM	577	N	LEU	A	452	7.694	3.779	26.968	1.00	2.00	N
ATOM	578	CA	LEU	A	452	8.787	2.978	27.445	1.00	2.00	C
ATOM	579	CB	LEU	A	452	9.493	2.241	26.276	1.00	2.00	C
ATOM	580	CG	LEU	A	452	9.745	0.778	26.453	1.00	3.02	C
ATOM	581	CD1	LEU	A	452	10.674	0.419	25.328	1.00	5.79	C
ATOM	582	CD2	LEU	A	452	10.172	0.204	27.937	1.00	2.00	C
ATOM	583	C	LEU	A	452	9.821	3.895	28.051	1.00	2.00	C
ATOM	584	O	LEU	A	452	10.339	3.642	29.139	1.00	2.00	O
ATOM	585	N	TYR	A	453	10.108	4.944	27.287	1.00	2.78	N
ATOM	586	CA	TYR	A	453	11.061	6.011	27.640	1.00	3.85	C
ATOM	587	CB	TYR	A	453	10.910	7.176	26.662	1.00	3.22	C
ATOM	588	CG	TYR	A	453	11.501	8.535	27.070	1.00	2.74	C
ATOM	589	CD1	TYR	A	453	12.868	8.741	27.164	1.00	2.00	C
ATOM	590	CE1	TYR	A	453	13.402	9.990	27.425	1.00	2.00	C
ATOM	591	CZ	TYR	A	453	12.543	11.062	27.581	1.00	2.98	C
ATOM	592	OH	TYR	A	453	12.996	12.386	27.820	1.00	2.14	O
ATOM	593	CE2	TYR	A	453	11.177	10.869	27.486	1.00	2.00	C
ATOM	594	CD2	TYR	A	453	10.675	9.642	27.209	1.00	2.00	C
ATOM	595	C	TYR	A	453	10.847	6.521	29.061	1.00	2.90	C
ATOM	596	O	TYR	A	453	11.761	6.551	29.867	1.00	2.00	O
ATOM	597	N	TYR	A	454	9.603	6.875	29.346	1.00	2.73	N
ATOM	598	CA	TYR	A	454	9.261	7.371	30.661	1.00	2.78	C
ATOM	599	CB	TYR	A	454	7.886	8.025	30.665	1.00	2.00	C
ATOM	600	CG	TYR	A	454	7.875	9.427	30.084	1.00	2.00	C
ATOM	601	CD1	TYR	A	454	8.920	10.320	30.330	1.00	5.16	C
ATOM	602	CE1	TYR	A	454	8.888	11.674	29.835	1.00	2.49	C

ATOM	603	CZ	TYR	A	454	7.841	12.047	29.107	1.00	2.99	C
ATOM	604	OH	TYR	A	454	7.794	13.303	28.578	1.00	3.52	O
ATOM	605	CE2	TYR	A	454	6.795	11.146	28.853	1.00	4.23	C
ATOM	606	CD2	TYR	A	454	6.842	9.862	29.328	1.00	2.00	C
ATOM	607	C	TYR	A	454	9.367	6.274	31.709	1.00	3.50	C
ATOM	608	O	TYR	A	454	9.906	6.509	32.803	1.00	4.53	O
ATOM	609	N	ARG	A	455	8.870	5.080	31.388	1.00	3.34	N
ATOM	610	CA	ARG	A	455	8.891	3.972	32.323	1.00	3.12	C
ATOM	611	CB	ARG	A	455	8.101	2.818	31.725	1.00	3.07	C
ATOM	612	CG	ARG	A	455	8.180	1.507	32.471	1.00	2.58	C
ATOM	613	CD	ARG	A	455	7.680	0.344	31.669	1.00	2.00	C
ATOM	614	NE	ARG	A	455	8.236	-0.942	32.090	1.00	6.42	N
ATOM	615	CZ	ARG	A	455	7.807	-1.662	33.179	1.00	11.99	C
ATOM	616	NH1	ARG	A	455	8.348	-2.862	33.469	1.00	9.20	N
ATOM	617	NH2	ARG	A	455	6.802	-1.218	33.939	1.00	9.54	N
ATOM	618	C	ARG	A	455	10.365	3.589	32.710	1.00	4.18	C
ATOM	619	O	ARG	A	455	10.681	3.275	33.841	1.00	5.50	O
ATOM	620	N	VAL	A	456	11.282	3.706	31.771	1.00	4.54	N
ATOM	621	CA	VAL	A	456	12.683	3.420	31.981	1.00	2.65	C
ATOM	622	CB	VAL	A	456	13.312	3.113	30.643	1.00	2.00	C
ATOM	623	CG1	VAL	A	456	14.859	3.065	30.755	1.00	4.98	C
ATOM	624	CG2	VAL	A	456	12.742	1.787	30.107	1.00	2.00	C
ATOM	625	C	VAL	A	456	13.432	4.511	32.717	1.00	2.66	C
ATOM	626	O	VAL	A	456	14.296	4.238	33.552	1.00	3.62	O
ATOM	627	N	MET	A	457	13.107	5.760	32.430	1.00	3.27	N
ATOM	628	CA	MET	A	457	13.752	6.909	33.073	1.00	2.00	C
ATOM	629	CB	MET	A	457	13.250	8.218	32.443	1.00	2.00	C
ATOM	630	CG	MET	A	457	13.849	9.459	33.049	1.00	2.00	C
ATOM	631	SD	MET	A	457	13.120	11.027	32.572	1.00	2.00	S
ATOM	632	CE	MET	A	457	13.434	10.941	30.705	1.00	2.00	C
ATOM	633	C	MET	A	457	13.454	6.866	34.580	1.00	2.43	C
ATOM	634	O	MET	A	457	14.312	7.094	35.376	1.00	2.00	O
ATOM	635	N	GLU	A	458	12.217	6.546	34.941	1.00	3.37	N
ATOM	636	CA	GLU	A	458	11.796	6.489	36.329	1.00	4.85	C
ATOM	637	CB	GLU	A	458	10.250	6.508	36.461	1.00	6.22	C
ATOM	638	CG	GLU	A	458	9.743	6.297	37.876	1.00	9.88	C
ATOM	639	CD	GLU	A	458	8.217	6.296	38.008	1.00	16.41	C
ATOM	640	OE1	GLU	A	458	7.728	6.142	39.145	1.00	16.60	O

ATOM	641	OE2	GLU	A	458	7.494	6.470	36.992	1.00	21.88	O
ATOM	642	C	GLU	A	458	12.397	5.295	37.024	1.00	3.62	C
ATOM	643	O	GLU	A	458	12.707	5.380	38.188	1.00	2.58	O
ATOM	644	N	SER	A	459	12.607	4.189	36.300	1.00	3.61	N
ATOM	645	CA	SER	A	459	13.252	3.018	36.912	1.00	2.73	C
ATOM	646	CB	SER	A	459	13.078	1.796	36.043	1.00	2.08	C
ATOM	647	OG	SER	A	459	13.733	0.633	36.548	1.00	2.00	O
ATOM	648	C	SER	A	459	14.736	3.330	37.168	1.00	3.70	C
ATOM	649	O	SER	A	459	15.297	2.986	38.201	1.00	2.47	O
ATOM	650	N	MET	A	460	15.368	4.020	36.230	1.00	4.07	N
ATOM	651	CA	MET	A	460	16.754	4.383	36.433	1.00	4.93	C
ATOM	652	CB	MET	A	460	17.361	5.054	35.178	1.00	4.86	C
ATOM	653	CG	MET	A	460	17.501	4.164	33.993	1.00	8.07	C
ATOM	654	SD	MET	A	460	18.246	4.959	32.523	1.00	13.32	S
ATOM	655	CE	MET	A	460	18.698	3.528	31.591	1.00	10.36	C
ATOM	656	C	MET	A	460	16.909	5.320	37.641	1.00	5.63	C
ATOM	657	O	MET	A	460	17.854	5.152	38.423	1.00	5.63	O
ATOM	658	N	LEU	A	461	16.023	6.318	37.767	1.00	5.49	N
ATOM	659	CA	LEU	A	461	16.142	7.295	38.821	1.00	6.56	C
ATOM	660	CB	LEU	A	461	15.134	8.436	38.604	1.00	6.42	C
ATOM	661	CG	LEU	A	461	15.377	9.443	37.446	1.00	6.02	C
ATOM	662	CD1	LEU	A	461	14.169	10.331	37.283	1.00	2.12	C
ATOM	663	CD2	LEU	A	461	16.678	10.249	37.573	1.00	2.00	C
ATOM	664	C	LEU	A	461	15.932	6.630	40.218	1.00	8.27	C
ATOM	665	O	LEU	A	461	16.665	6.892	41.159	1.00	7.16	O
ATOM	666	N	LYS	A	462	14.903	5.799	40.351	1.00	10.76	N
ATOM	667	CA	LYS	A	462	14.653	5.106	41.623	1.00	13.62	C
ATOM	668	CB	LYS	A	462	13.464	4.156	41.578	1.00	13.89	C
ATOM	669	CG	LYS	A	462	12.086	4.865	41.307	1.00	17.14	C
ATOM	670	CD	LYS	A	462	10.931	3.852	41.398	1.00	20.36	C
ATOM	671	CE	LYS	A	462	9.546	4.493	41.278	1.00	19.96	C
ATOM	672	NZ	LYS	A	462	8.469	3.509	41.729	1.00	17.73	N
ATOM	673	C	LYS	A	462	15.886	4.330	41.985	1.00	13.79	C
ATOM	674	O	LYS	A	462	16.346	4.384	43.137	1.00	15.92	O
ATOM	675	N	SER	A	463	16.491	3.733	40.987	1.00	12.72	N
ATOM	676	CA	SER	A	463	17.684	2.995	41.195	1.00	13.57	C
ATOM	677	CB	SER	A	463	18.055	2.288	39.926	1.00	14.00	C
ATOM	678	OG	SER	A	463	19.089	1.391	40.192	1.00	13.63	O

ATOM	679	C	SER	A	463	18.862	3.837	41.628	1.00	14.52	C
ATOM	680	O	SER	A	463	19.609	3.479	42.533	1.00	15.99	O
ATOM	681	N	GLU	A	464	19.070	4.958	40.971	1.00	14.97	N
ATOM	682	CA	GLU	A	464	20.196	5.767	41.321	1.00	14.47	C
ATOM	683	CB	GLU	A	464	20.352	6.912	40.359	1.00	13.37	C
ATOM	684	CG	GLU	A	464	21.027	6.509	39.072	1.00	15.00	C
ATOM	685	CD	GLU	A	464	22.427	5.984	39.244	1.00	13.58	C
ATOM	686	OE1	GLU	A	464	22.561	5.003	39.965	1.00	17.87	O
ATOM	687	OE2	GLU	A	464	23.388	6.526	38.654	1.00	12.54	O
ATOM	688	C	GLU	A	464	20.064	6.271	42.729	1.00	15.03	C
ATOM	689	O	GLU	A	464	21.057	6.362	43.440	1.00	13.80	O
ATOM	690	N	GLU	A	465	18.835	6.619	43.107	1.00	16.34	N
ATOM	691	CA	GLU	A	465	18.551	7.176	44.428	1.00	18.04	C
ATOM	692	CB	GLU	A	465	17.056	7.574	44.544	1.00	17.67	C
ATOM	693	CG	GLU	A	465	16.680	8.192	45.889	1.00	19.26	C
ATOM	694	CD	GLU	A	465	15.185	8.431	46.085	1.00	21.39	C
ATOM	695	OE1	GLU	A	465	14.733	8.538	47.260	1.00	24.00	O
ATOM	696	OE2	GLU	A	465	14.460	8.543	45.086	1.00	20.75	O
ATOM	697	C	GLU	A	465	18.981	6.218	45.554	1.00	18.80	C
ATOM	698	O	GLU	A	465	19.486	6.627	46.552	1.00	18.58	O
ATOM	699	N	GLU	A	466	18.818	4.922	45.356	1.00	21.36	N
ATOM	700	CA	GLU	A	466	19.154	3.978	46.399	1.00	23.94	C
ATOM	701	CB	GLU	A	466	18.257	2.740	46.301	1.00	24.78	C
ATOM	702	CG	GLU	A	466	18.800	1.694	45.376	1.00	31.30	C
ATOM	703	CD	GLU	A	466	18.024	0.404	45.467	1.00	37.63	C
ATOM	704	OE1	GLU	A	466	17.805	-0.006	46.641	1.00	39.08	O
ATOM	705	OE2	GLU	A	466	17.638	-0.157	44.382	1.00	36.89	O
ATOM	706	C	GLU	A	466	20.600	3.578	46.356	1.00	23.81	C
ATOM	707	O	GLU	A	466	21.106	2.912	47.247	1.00	23.07	O
ATOM	708	N	ARG	A	467	21.257	3.973	45.272	1.00	25.21	N
ATOM	709	CA	ARG	A	467	22.666	3.659	45.051	1.00	24.44	C
ATOM	710	CB	ARG	A	467	22.925	3.465	43.576	1.00	23.48	C
ATOM	711	CG	ARG	A	467	24.352	3.283	43.224	1.00	21.88	C
ATOM	712	CD	ARG	A	467	24.659	3.512	41.707	1.00	20.93	C
ATOM	713	NE	ARG	A	467	26.015	4.022	41.616	1.00	18.63	N
ATOM	714	CZ	ARG	A	467	26.367	5.089	40.982	1.00	15.74	C
ATOM	715	NH1	ARG	A	467	25.481	5.760	40.281	1.00	12.88	N
ATOM	716	NH2	ARG	A	467	27.641	5.467	41.027	1.00	18.41	N

ATOM	717	C	ARG	A	467	23.560	4.765	45.573	1.00 24.26	C
ATOM	718	O	ARG	A	467	24.669	4.516	45.988	1.00 25.68	O
ATOM	719	N	LEU	A	468	23.067	5.979	45.572	1.00 23.45	N
ATOM	720	CA	LEU	A	468	23.871	7.109	45.983	1.00 23.85	C
ATOM	721	CB	LEU	A	468	24.092	8.052	44.801	1.00 23.40	C
ATOM	722	CG	LEU	A	468	24.921	7.685	43.581	1.00 23.39	C
ATOM	723	CD1	LEU	A	468	24.393	8.459	42.390	1.00 19.92	C
ATOM	724	CD2	LEU	A	468	26.380	8.047	43.836	1.00 25.54	C
ATOM	725	C	LEU	A	468	23.174	7.919	47.087	1.00 24.22	C
ATOM	726	O	LEU	A	468	23.753	8.862	47.608	1.00 23.40	O
ATOM	727	N	SER	A	469	21.940	7.549	47.427	1.00 24.43	N
ATOM	728	CA	SER	A	469	21.160	8.357	48.310	1.00 25.52	C
ATOM	729	CB	SER	A	469	21.893	8.580	49.621	1.00 26.28	C
ATOM	730	OG	SER	A	469	22.034	7.352	50.339	1.00 24.93	O
ATOM	731	C	SER	A	469	21.022	9.644	47.500	1.00 26.91	C
ATOM	732	O	SER	A	469	21.227	9.627	46.285	1.00 28.46	O
ATOM	733	N	ILE	A	470	20.666	10.774	48.091	1.00 26.91	N
ATOM	734	CA	ILE	A	470	20.567	11.941	47.218	1.00 25.86	C
ATOM	735	CB	ILE	A	470	21.907	12.106	46.458	1.00 25.79	C
ATOM	736	CG1	ILE	A	470	22.706	13.245	47.112	1.00 26.46	C
ATOM	737	CD1	ILE	A	470	24.137	13.426	46.636	1.00 28.15	C
ATOM	738	CG2	ILE	A	470	21.697	12.313	44.944	1.00 25.97	C
ATOM	739	C	ILE	A	470	19.406	11.815	46.260	1.00 25.84	C
ATOM	740	O	ILE	A	470	19.196	10.760	45.661	1.00 23.67	O
ATOM	741	N	GLN	A	471	18.600	12.878	46.174	1.00 26.30	N
ATOM	742	CA	GLN	A	471	17.516	12.894	45.210	1.00 27.70	C
ATOM	743	CB	GLN	A	471	16.221	13.383	45.835	1.00 28.63	C
ATOM	744	CG	GLN	A	471	15.514	12.376	46.723	1.00 32.75	C
ATOM	745	CD	GLN	A	471	16.285	12.086	48.043	1.00 38.95	C
ATOM	746	OE1	GLN	A	471	16.536	13.000	48.845	1.00 36.46	O
ATOM	747	NE2	GLN	A	471	16.656	10.801	48.257	1.00 41.47	N
ATOM	748	C	GLN	A	471	18.005	13.851	44.141	1.00 27.03	C
ATOM	749	O	GLN	A	471	19.174	13.799	43.776	1.00 28.39	O
ATOM	750	N	ASN	A	472	17.163	14.703	43.585	1.00 25.58	N
ATOM	751	CA	ASN	A	472	17.755	15.736	42.680	1.00 25.14	C
ATOM	752	CB	ASN	A	472	18.985	16.425	43.345	1.00 24.93	C
ATOM	753	CG	ASN	A	472	19.348	17.803	42.708	1.00 28.30	C
ATOM	754	OD1	ASN	A	472	19.877	18.682	43.390	1.00 23.38	O

ATOM	755	ND2	ASN	A	472	19.073	17.974	41.391	1.00	29.82	N
ATOM	756	C	ASN	A	472	18.118	15.198	41.256	1.00	22.63	C
ATOM	757	O	ASN	A	472	17.204	14.902	40.446	1.00	21.83	O
ATOM	758	N	PHE	A	473	19.419	15.043	40.990	1.00	19.00	N
ATOM	759	CA	PHE	A	473	19.885	14.539	39.654	1.00	17.56	C
ATOM	760	CB	PHE	A	473	19.095	13.278	39.175	1.00	15.51	C
ATOM	761	CG	PHE	A	473	19.295	12.095	40.041	1.00	14.08	C
ATOM	762	CD1	PHE	A	473	18.379	11.788	41.031	1.00	14.53	C
ATOM	763	CE1	PHE	A	473	18.603	10.715	41.900	1.00	11.36	C
ATOM	764	CZ	PHE	A	473	19.726	9.961	41.785	1.00	8.01	C
ATOM	765	CE2	PHE	A	473	20.648	10.257	40.810	1.00	10.92	C
ATOM	766	CD2	PHE	A	473	20.444	11.329	39.954	1.00	13.01	C
ATOM	767	C	PHE	A	473	19.944	15.623	38.527	1.00	15.68	C
ATOM	768	O	PHE	A	473	20.018	15.264	37.360	1.00	15.69	O
ATOM	769	N	SER	A	474	19.930	16.910	38.897	1.00	13.72	N
ATOM	770	CA	SER	A	474	19.840	18.016	37.936	1.00	13.11	C
ATOM	771	CB	SER	A	474	20.136	19.379	38.604	1.00	14.23	C
ATOM	772	OG	SER	A	474	19.705	20.550	37.894	1.00	6.19	O
ATOM	773	C	SER	A	474	20.702	17.877	36.691	1.00	13.44	C
ATOM	774	O	SER	A	474	20.221	18.062	35.597	1.00	13.49	O
ATOM	775	N	LYS	A	475	21.978	17.578	36.867	1.00	13.37	N
ATOM	776	CA	LYS	A	475	22.878	17.435	35.754	1.00	12.47	C
ATOM	777	CB	LYS	A	475	24.286	17.089	36.185	1.00	12.77	C
ATOM	778	CG	LYS	A	475	25.288	17.204	35.033	1.00	13.73	C
ATOM	779	CD	LYS	A	475	26.724	17.423	35.480	1.00	16.66	C
ATOM	780	CE	LYS	A	475	27.742	17.332	34.315	1.00	24.37	C
ATOM	781	NZ	LYS	A	475	27.400	18.006	32.937	1.00	23.53	N
ATOM	782	C	LYS	A	475	22.467	16.436	34.747	1.00	12.94	C
ATOM	783	O	LYS	A	475	22.438	16.736	33.530	1.00	14.20	O
ATOM	784	N	LEU	A	476	22.188	15.223	35.203	1.00	12.84	N
ATOM	785	CA	LEU	A	476	21.832	14.124	34.294	1.00	11.68	C
ATOM	786	CB	LEU	A	476	21.567	12.879	35.056	1.00	11.55	C
ATOM	787	CG	LEU	A	476	21.072	11.659	34.255	1.00	14.10	C
ATOM	788	CD1	LEU	A	476	21.999	11.262	33.212	1.00	12.17	C
ATOM	789	CD2	LEU	A	476	20.899	10.436	35.250	1.00	14.83	C
ATOM	790	C	LEU	A	476	20.597	14.474	33.514	1.00	11.27	C
ATOM	791	O	LEU	A	476	20.608	14.449	32.289	1.00	11.58	O
ATOM	792	N	LEU	A	477	19.554	14.876	34.234	1.00	9.67	N

ATOM	793	CA	LEU	A	477	18.271	15.210	33.633	1.00	7.27	C
ATOM	794	CB	LEU	A	477	17.211	15.256	34.724	1.00	6.59	C
ATOM	795	CG	LEU	A	477	17.000	13.934	35.430	1.00	6.22	C
ATOM	796	CD1	LEU	A	477	15.877	14.102	36.533	1.00	2.69	C
ATOM	797	CD2	LEU	A	477	16.667	12.908	34.367	1.00	2.00	C
ATOM	798	C	LEU	A	477	18.236	16.520	32.794	1.00	6.03	C
ATOM	799	O	LEU	A	477	17.234	16.807	32.164	1.00	5.74	O
ATOM	800	N	ASN	A	478	19.283	17.310	32.784	1.00	4.35	N
ATOM	801	CA	ASN	A	478	19.264	18.470	31.877	1.00	6.17	C
ATOM	802	CB	ASN	A	478	19.716	19.783	32.539	1.00	5.15	C
ATOM	803	CG	ASN	A	478	18.612	20.397	33.419	1.00	5.45	C
ATOM	804	OD1	ASN	A	478	17.615	20.849	32.868	1.00	6.20	O
ATOM	805	ND2	ASN	A	478	18.764	20.374	34.773	1.00	2.00	N
ATOM	806	C	ASN	A	478	20.057	18.257	30.562	1.00	6.46	C
ATOM	807	O	ASN	A	478	20.037	19.127	29.680	1.00	6.14	O
ATOM	808	N	ASP	A	479	20.712	17.098	30.461	1.00	5.99	N
ATOM	809	CA	ASP	A	479	21.572	16.766	29.360	1.00	7.55	C
ATOM	810	CB	ASP	A	479	22.520	15.643	29.755	1.00	7.69	C
ATOM	811	CG	ASP	A	479	23.519	15.344	28.706	1.00	12.13	C
ATOM	812	OD1	ASP	A	479	23.206	15.086	27.511	1.00	18.57	O
ATOM	813	OD2	ASP	A	479	24.708	15.317	28.984	1.00	21.87	O
ATOM	814	C	ASP	A	479	20.791	16.305	28.146	1.00	7.54	C
ATOM	815	O	ASP	A	479	20.205	15.236	28.165	1.00	8.94	O
ATOM	816	N	ASN	A	480	20.893	17.062	27.063	1.00	6.80	N
ATOM	817	CA	ASN	A	480	20.198	16.762	25.841	1.00	5.52	C
ATOM	818	CB	ASN	A	480	20.510	17.835	24.799	1.00	4.25	C
ATOM	819	CG	ASN	A	480	19.772	17.630	23.540	1.00	5.64	C
ATOM	820	OD1	ASN	A	480	20.369	17.413	22.488	1.00	13.62	O
ATOM	821	ND2	ASN	A	480	18.463	17.638	23.620	1.00	5.94	N
ATOM	822	C	ASN	A	480	20.522	15.352	25.332	1.00	4.85	C
ATOM	823	O	ASN	A	480	19.612	14.554	25.048	1.00	2.00	O
ATOM	824	N	ILE	A	481	21.812	15.051	25.262	1.00	5.91	N
ATOM	825	CA	ILE	A	481	22.281	13.726	24.790	1.00	6.95	C
ATOM	826	CB	ILE	A	481	23.805	13.604	24.829	1.00	7.62	C
ATOM	827	CG1	ILE	A	481	24.480	14.691	23.972	1.00	8.74	C
ATOM	828	CD1	ILE	A	481	24.208	14.429	22.466	1.00	17.85	C
ATOM	829	CG2	ILE	A	481	24.205	12.265	24.282	1.00	7.84	C
ATOM	830	C	ILE	A	481	21.713	12.560	25.551	1.00	6.93	C

ATOM	831	O	ILE	A	481	21.364	11.555	24.932	1.00	8.37	O
ATOM	832	N	PHE	A	482	21.656	12.660	26.879	1.00	5.61	N
ATOM	833	CA	PHE	A	482	21.076	11.595	27.710	1.00	4.96	C
ATOM	834	CB	PHE	A	482	21.064	11.967	29.220	1.00	3.95	C
ATOM	835	CG	PHE	A	482	20.218	11.064	30.044	1.00	2.00	C
ATOM	836	CD1	PHE	A	482	20.616	9.760	30.273	1.00	2.30	C
ATOM	837	CE1	PHE	A	482	19.779	8.872	31.037	1.00	4.02	C
ATOM	838	CZ	PHE	A	482	18.537	9.353	31.571	1.00	6.39	C
ATOM	839	CE2	PHE	A	482	18.140	10.701	31.307	1.00	3.09	C
ATOM	840	CD2	PHE	A	482	18.986	11.517	30.569	1.00	2.00	C
ATOM	841	C	PHE	A	482	19.631	11.205	27.303	1.00	4.81	C
ATOM	842	O	PHE	A	482	19.379	10.044	27.144	1.00	4.61	O
ATOM	843	N	HIS	A	483	18.721	12.184	27.192	1.00	3.46	N
ATOM	844	CA	HIS	A	483	17.323	11.995	26.803	1.00	4.48	C
ATOM	845	CB	HIS	A	483	16.500	13.264	27.001	1.00	3.03	C
ATOM	846	CG	HIS	A	483	16.343	13.637	28.434	1.00	6.88	C
ATOM	847	ND1	HIS	A	483	15.533	12.932	29.305	1.00	5.16	N
ATOM	848	CE1	HIS	A	483	15.629	13.475	30.504	1.00	6.16	C
ATOM	849	NE2	HIS	A	483	16.479	14.482	30.451	1.00	4.45	N
ATOM	850	CD2	HIS	A	483	16.956	14.590	29.173	1.00	5.78	C
ATOM	851	C	HIS	A	483	17.210	11.610	25.339	1.00	4.68	C
ATOM	852	O	HIS	A	483	16.287	10.899	24.919	1.00	4.81	O
ATOM	853	N	MET	A	484	18.163	12.066	24.564	1.00	4.57	N
ATOM	854	CA	MET	A	484	18.143	11.733	23.163	1.00	5.49	C
ATOM	855	CB	MET	A	484	19.135	12.555	22.454	1.00	5.43	C
ATOM	856	CG	MET	A	484	18.627	13.127	21.223	1.00	13.21	C
ATOM	857	SD	MET	A	484	17.108	14.107	21.275	1.00	15.95	S
ATOM	858	CE	MET	A	484	17.888	15.586	21.607	1.00	23.47	C
ATOM	859	C	MET	A	484	18.512	10.264	23.026	1.00	4.72	C
ATOM	860	O	MET	A	484	17.927	9.590	22.188	1.00	4.49	O
ATOM	861	N	SER	A	485	19.399	9.758	23.892	1.00	2.84	N
ATOM	862	CA	SER	A	485	19.863	8.378	23.799	1.00	3.18	C
ATOM	863	CB	SER	A	485	21.196	8.206	24.505	1.00	4.17	C
ATOM	864	OG	SER	A	485	22.253	8.922	23.891	1.00	5.43	O
ATOM	865	C	SER	A	485	18.866	7.382	24.382	1.00	2.76	C
ATOM	866	O	SER	A	485	18.580	6.323	23.797	1.00	3.40	O
ATOM	867	N	LEU	A	486	18.291	7.753	25.499	1.00	2.70	N
ATOM	868	CA	LEU	A	486	17.294	6.932	26.173	1.00	2.83	C

ATOM	869	CB	LEU	A	486	16.795	7.645	27.456	1.00	2.69	C
ATOM	870	CG	LEU	A	486	16.678	6.926	28.798	1.00	5.49	C
ATOM	871	CD1	LEU	A	486	15.484	7.415	29.632	1.00	2.00	C
ATOM	872	CD2	LEU	A	486	16.643	5.426	28.695	1.00	7.92	C
ATOM	873	C	LEU	A	486	16.135	6.698	25.188	1.00	2.25	C
ATOM	874	O	LEU	A	486	15.750	5.566	24.970	1.00	2.40	O
ATOM	875	N	LEU	A	487	15.645	7.774	24.562	1.00	2.00	N
ATOM	876	CA	LEU	A	487	14.480	7.731	23.690	1.00	3.45	C
ATOM	877	CB	LEU	A	487	14.104	9.150	23.196	1.00	4.14	C
ATOM	878	CG	LEU	A	487	12.637	9.614	23.068	1.00	5.86	C
ATOM	879	CD1	LEU	A	487	12.505	10.719	21.953	1.00	4.99	C
ATOM	880	CD2	LEU	A	487	11.658	8.512	22.759	1.00	7.08	C
ATOM	881	C	LEU	A	487	14.718	6.785	22.477	1.00	3.80	C
ATOM	882	O	LEU	A	487	13.887	5.903	22.194	1.00	2.00	O
ATOM	883	N	ALA	A	488	15.873	6.983	21.838	1.00	3.28	N
ATOM	884	CA	ALA	A	488	16.299	6.192	20.698	1.00	4.99	C
ATOM	885	CB	ALA	A	488	17.695	6.594	20.270	1.00	5.66	C
ATOM	886	C	ALA	A	488	16.341	4.758	21.092	1.00	5.49	C
ATOM	887	O	ALA	A	488	15.806	3.885	20.441	1.00	6.07	O
ATOM	888	N	CYS	A	489	16.993	4.496	22.198	1.00	6.10	N
ATOM	889	CA	CYS	A	489	17.122	3.122	22.588	1.00	5.29	C
ATOM	890	CB	CYS	A	489	17.998	3.023	23.837	1.00	4.37	C
ATOM	891	SG	CYS	A	489	18.230	1.310	24.279	1.00	5.78	S
ATOM	892	C	CYS	A	489	15.738	2.513	22.729	1.00	5.44	C
ATOM	893	O	CYS	A	489	15.444	1.438	22.163	1.00	4.75	O
ATOM	894	N	ALA	A	490	14.888	3.233	23.462	1.00	5.61	N
ATOM	895	CA	ALA	A	490	13.503	2.829	23.673	1.00	5.43	C
ATOM	896	CB	ALA	A	490	12.815	3.780	24.604	1.00	6.08	C
ATOM	897	C	ALA	A	490	12.700	2.669	22.406	1.00	4.62	C
ATOM	898	O	ALA	A	490	11.860	1.779	22.335	1.00	6.60	O
ATOM	899	N	LEU	A	491	12.957	3.472	21.395	1.00	3.23	N
ATOM	900	CA	LEU	A	491	12.237	3.330	20.140	1.00	2.52	C
ATOM	901	CB	LEU	A	491	12.343	4.622	19.349	1.00	2.72	C
ATOM	902	CG	LEU	A	491	11.536	5.885	19.661	1.00	2.48	C
ATOM	903	CD1	LEU	A	491	12.083	7.153	18.984	1.00	2.00	C
ATOM	904	CD2	LEU	A	491	10.047	5.660	19.324	1.00	2.00	C
ATOM	905	C	LEU	A	491	12.851	2.178	19.332	1.00	3.77	C
ATOM	906	O	LEU	A	491	12.243	1.614	18.485	1.00	3.11	O

ATOM	907	N	GLU	A	492	14.109	1.865	19.555	1.00	5.20	N
ATOM	908	CA	GLU	A	492	14.694	0.850	18.745	1.00	7.70	C
ATOM	909	CB	GLU	A	492	16.201	0.864	18.909	1.00	7.57	C
ATOM	910	CG	GLU	A	492	16.964	-0.236	18.193	1.00	10.36	C
ATOM	911	CD	GLU	A	492	16.581	-0.371	16.735	1.00	12.45	C
ATOM	912	OE1	GLU	A	492	16.431	0.631	16.081	1.00	17.37	O
ATOM	913	OE2	GLU	A	492	16.433	-1.468	16.213	1.00	14.99	O
ATOM	914	C	GLU	A	492	14.102	-0.480	19.162	1.00	9.34	C
ATOM	915	O	GLU	A	492	13.919	-1.384	18.346	1.00	9.42	O
ATOM	916	N	VAL	A	493	13.806	-0.597	20.445	1.00	10.25	N
ATOM	917	CA	VAL	A	493	13.230	-1.804	20.970	1.00	10.00	C
ATOM	918	CB	VAL	A	493	13.208	-1.735	22.536	1.00	11.55	C
ATOM	919	CG1	VAL	A	493	12.173	-2.764	23.129	1.00	8.23	C
ATOM	920	CG2	VAL	A	493	14.608	-1.955	23.072	1.00	7.40	C
ATOM	921	C	VAL	A	493	11.802	-1.988	20.466	1.00	10.30	C
ATOM	922	O	VAL	A	493	11.449	-3.037	20.047	1.00	10.69	O
ATOM	923	N	VAL	A	494	11.016	-0.926	20.434	1.00	10.67	N
ATOM	924	CA	VAL	A	494	9.637	-1.000	20.006	1.00	10.15	C
ATOM	925	CB	VAL	A	494	8.838	0.337	20.293	1.00	9.64	C
ATOM	926	CG1	VAL	A	494	7.530	0.329	19.610	1.00	6.54	C
ATOM	927	CG2	VAL	A	494	8.558	0.545	21.852	1.00	6.43	C
ATOM	928	C	VAL	A	494	9.550	-1.362	18.563	1.00	12.13	C
ATOM	929	O	VAL	A	494	8.754	-2.219	18.178	1.00	12.62	O
ATOM	930	N	MET	A	495	10.363	-0.722	17.742	1.00	13.37	N
ATOM	931	CA	MET	A	495	10.344	-1.038	16.324	1.00	15.28	C
ATOM	932	CB	MET	A	495	11.097	0.035	15.531	1.00	14.65	C
ATOM	933	CG	MET	A	495	10.405	1.316	15.544	1.00	13.27	C
ATOM	934	SD	MET	A	495	11.314	2.329	14.534	1.00	18.39	S
ATOM	935	CE	MET	A	495	10.911	1.751	12.891	1.00	23.19	C
ATOM	936	C	MET	A	495	10.876	-2.438	15.991	1.00	16.42	C
ATOM	937	O	MET	A	495	10.586	-2.968	14.935	1.00	15.60	O
ATOM	938	N	ALA	A	496	11.688	-2.993	16.884	1.00	18.74	N
ATOM	939	CA	ALA	A	496	12.290	-4.310	16.687	1.00	21.16	C
ATOM	940	CB	ALA	A	496	13.319	-4.623	17.755	1.00	20.54	C
ATOM	941	C	ALA	A	496	11.219	-5.344	16.778	1.00	23.00	C
ATOM	942	O	ALA	A	496	11.094	-6.267	15.922	1.00	22.03	O
ATOM	943	N	THR	A	497	10.445	-5.221	17.836	1.00	24.64	N
ATOM	944	CA	THR	A	497	9.436	-6.220	18.009	1.00	27.98	C

ATOM	945	CB	THR	A	497	8.657	-5.942	19.223	1.00	27.33	C
ATOM	946	OG1	THR	A	497	7.876	-4.776	18.968	1.00	29.40	O
ATOM	947	CG2	THR	A	497	9.609	-5.593	20.366	1.00	25.14	C
ATOM	948	C	THR	A	497	8.512	-6.334	16.784	1.00	30.44	C
ATOM	949	O	THR	A	497	8.060	-7.443	16.457	1.00	30.05	O
ATOM	950	N	TYR	A	498	8.256	-5.210	16.104	1.00	33.44	N
ATOM	951	CA	TYR	A	498	7.368	-5.204	14.927	1.00	36.84	C
ATOM	952	CB	TYR	A	498	6.363	-4.042	14.984	1.00	36.22	C
ATOM	953	CG	TYR	A	498	5.695	-3.904	16.329	1.00	37.40	C
ATOM	954	CD1	TYR	A	498	4.755	-4.822	16.756	1.00	39.74	C
ATOM	955	CE1	TYR	A	498	4.162	-4.693	18.018	1.00	41.01	C
ATOM	956	CZ	TYR	A	498	4.520	-3.631	18.828	1.00	38.06	C
ATOM	957	OH	TYR	A	498	3.974	-3.454	20.077	1.00	38.69	O
ATOM	958	CE2	TYR	A	498	5.443	-2.731	18.404	1.00	35.90	C
ATOM	959	CD2	TYR	A	498	6.019	-2.865	17.183	1.00	35.68	C
ATOM	960	C	TYR	A	498	8.074	-5.242	13.556	1.00	39.17	C
ATOM	961	O	TYR	A	498	7.561	-4.693	12.563	1.00	40.64	O
ATOM	962	N	SER	A	499	9.233	-5.887	13.478	1.00	41.51	N
ATOM	963	CA	SER	A	499	9.962	-5.935	12.205	1.00	43.56	C
ATOM	964	CB	SER	A	499	11.290	-6.704	12.338	1.00	43.58	C
ATOM	965	OG	SER	A	499	12.305	-5.924	12.951	1.00	41.96	O
ATOM	966	C	SER	A	499	9.098	-6.527	11.084	1.00	45.17	C
ATOM	967	O	SER	A	499	9.103	-5.993	9.973	1.00	45.09	O
ATOM	968	N	ARG	A	500	8.382	-7.631	11.378	1.00	46.76	N
ATOM	969	CA	ARG	A	500	7.476	-8.292	10.409	1.00	48.01	C
ATOM	970	CB	ARG	A	500	7.233	-9.738	10.797	1.00	47.71	C
ATOM	971	CG	ARG	A	500	6.773	-10.619	9.631	1.00	49.22	C
ATOM	972	CD	ARG	A	500	5.473	-11.420	9.915	1.00	50.50	C
ATOM	973	NE	ARG	A	500	4.297	-10.547	10.020	1.00	52.41	N
ATOM	974	CZ	ARG	A	500	3.024	-10.961	10.043	1.00	52.33	C
ATOM	975	NH1	ARG	A	500	2.726	-12.270	9.976	1.00	49.40	N
ATOM	976	NH2	ARG	A	500	2.045	-10.052	10.132	1.00	49.92	N
ATOM	977	C	ARG	A	500	6.124	-7.563	10.321	1.00	48.87	C
ATOM	978	O	ARG	A	500	5.050	-8.171	10.489	1.00	48.55	O
ATOM	979	N	SER	A	501	6.211	-6.248	10.092	1.00	49.79	N
ATOM	980	CA	SER	A	501	5.058	-5.356	9.992	1.00	50.64	C
ATOM	981	CB	SER	A	501	5.166	-4.236	11.026	1.00	50.82	C
ATOM	982	OG	SER	A	501	4.077	-3.328	10.893	1.00	51.88	O

ATOM	983	C	SER	A	501	4.924	-4.738	8.587	1.00	50.90	C
ATOM	984	O	SER	A	501	3.844	-4.752	7.983	1.00	50.85	O
ATOM	985	N	SER	A	508	9.297	1.112	-0.283	1.00	57.14	N
ATOM	986	CA	SER	A	508	10.177	0.166	0.420	1.00	56.24	C
ATOM	987	CB	SER	A	508	10.072	-1.239	-0.219	1.00	56.13	C
ATOM	988	OG	SER	A	508	8.726	-1.704	-0.216	1.00	54.22	O
ATOM	989	C	SER	A	508	11.636	0.689	0.478	1.00	55.73	C
ATOM	990	O	SER	A	508	12.609	-0.084	0.559	1.00	56.00	O
ATOM	991	N	GLY	A	509	11.773	2.013	0.436	1.00	54.44	N
ATOM	992	CA	GLY	A	509	13.075	2.644	0.499	1.00	52.95	C
ATOM	993	C	GLY	A	509	13.712	2.435	1.851	1.00	51.71	C
ATOM	994	O	GLY	A	509	14.026	3.403	2.552	1.00	51.34	O
ATOM	995	N	THR	A	510	13.924	1.160	2.179	1.00	50.64	N
ATOM	996	CA	THR	A	510	14.498	0.702	3.455	1.00	49.39	C
ATOM	997	CB	THR	A	510	16.036	0.527	3.429	1.00	50.13	C
ATOM	998	OG1	THR	A	510	16.487	0.219	4.774	1.00	49.53	O
ATOM	999	CG2	THR	A	510	16.783	1.834	3.003	1.00	49.41	C
ATOM	1000	C	THR	A	510	14.164	1.482	4.674	1.00	48.11	C
ATOM	1001	O	THR	A	510	14.292	2.708	4.691	1.00	48.23	O
ATOM	1002	N	ASP	A	511	13.774	0.760	5.719	1.00	46.68	N
ATOM	1003	CA	ASP	A	511	13.456	1.400	6.998	1.00	44.62	C
ATOM	1004	CB	ASP	A	511	12.053	1.024	7.442	1.00	45.05	C
ATOM	1005	CG	ASP	A	511	11.752	1.485	8.823	1.00	44.34	C
ATOM	1006	OD1	ASP	A	511	11.716	2.709	9.062	1.00	47.00	O
ATOM	1007	OD2	ASP	A	511	11.556	0.693	9.743	1.00	43.18	O
ATOM	1008	C	ASP	A	511	14.454	1.018	8.093	1.00	42.93	C
ATOM	1009	O	ASP	A	511	15.641	0.716	7.827	1.00	42.65	O
ATOM	1010	N	LEU	A	512	13.953	1.009	9.322	1.00	40.19	N
ATOM	1011	CA	LEU	A	512	14.792	0.764	10.492	1.00	37.10	C
ATOM	1012	CB	LEU	A	512	13.935	0.548	11.720	1.00	36.88	C
ATOM	1013	CG	LEU	A	512	14.573	0.486	13.093	1.00	38.65	C
ATOM	1014	CD1	LEU	A	512	15.068	-0.968	13.429	1.00	39.66	C
ATOM	1015	CD2	LEU	A	512	15.676	1.573	13.278	1.00	39.27	C
ATOM	1016	C	LEU	A	512	15.743	-0.390	10.273	1.00	34.87	C
ATOM	1017	O	LEU	A	512	15.760	-1.031	9.220	1.00	34.35	O
ATOM	1018	N	SER	A	513	16.542	-0.607	11.299	1.00	32.30	N
ATOM	1019	CA	SER	A	513	17.599	-1.586	11.342	1.00	29.77	C
ATOM	1020	CB	SER	A	513	18.113	-1.943	9.931	1.00	30.70	C

ATOM	1021	OG	SER	A	513	17.245	-2.859	9.250	1.00	30.48	O
ATOM	1022	C	SER	A	513	18.597	-0.743	12.154	1.00	26.48	C
ATOM	1023	O	SER	A	513	19.360	0.031	11.624	1.00	25.26	O
ATOM	1024	N	PHE	A	514	18.537	-0.922	13.460	1.00	23.05	N
ATOM	1025	CA	PHE	A	514	19.332	-0.177	14.402	1.00	19.60	C
ATOM	1026	CB	PHE	A	514	20.495	-0.914	14.932	1.00	17.88	C
ATOM	1027	CG	PHE	A	514	21.410	-0.038	15.659	1.00	13.56	C
ATOM	1028	CD1	PHE	A	514	22.774	-0.135	15.466	1.00	7.78	C
ATOM	1029	CE1	PHE	A	514	23.601	0.675	16.127	1.00	7.61	C
ATOM	1030	CZ	PHE	A	514	23.077	1.632	17.011	1.00	10.61	C
ATOM	1031	CE2	PHE	A	514	21.715	1.743	17.219	1.00	5.65	C
ATOM	1032	CD2	PHE	A	514	20.893	0.919	16.539	1.00	7.37	C
ATOM	1033	C	PHE	A	514	19.831	1.160	13.883	1.00	19.98	C
ATOM	1034	O	PHE	A	514	19.175	2.200	14.198	1.00	21.97	O
ATOM	1035	N	PRO	A	515	20.917	1.189	13.071	1.00	16.87	N
ATOM	1036	CA	PRO	A	515	21.498	2.461	12.678	1.00	13.02	C
ATOM	1037	CB	PRO	A	515	22.506	2.056	11.613	1.00	13.72	C
ATOM	1038	CG	PRO	A	515	22.040	0.796	11.161	1.00	13.79	C
ATOM	1039	CD	PRO	A	515	21.587	0.062	12.404	1.00	16.21	C
ATOM	1040	C	PRO	A	515	20.449	3.495	12.185	1.00	11.10	C
ATOM	1041	O	PRO	A	515	20.673	4.693	12.490	1.00	11.58	O
ATOM	1042	N	TRP	A	516	19.356	3.097	11.514	1.00	8.08	N
ATOM	1043	CA	TRP	A	516	18.374	4.084	10.997	1.00	6.57	C
ATOM	1044	CB	TRP	A	516	17.119	3.393	10.446	1.00	6.20	C
ATOM	1045	CG	TRP	A	516	16.106	4.310	9.797	1.00	6.53	C
ATOM	1046	CD1	TRP	A	516	16.196	4.932	8.538	1.00	6.10	C
ATOM	1047	NE1	TRP	A	516	15.058	5.663	8.286	1.00	2.00	N
ATOM	1048	CE2	TRP	A	516	14.229	5.565	9.354	1.00	2.00	C
ATOM	1049	CD2	TRP	A	516	14.860	4.732	10.333	1.00	3.32	C
ATOM	1050	CE3	TRP	A	516	14.213	4.528	11.555	1.00	2.00	C
ATOM	1051	CZ3	TRP	A	516	12.976	5.088	11.741	1.00	2.00	C
ATOM	1052	CH2	TRP	A	516	12.376	5.861	10.761	1.00	2.00	C
ATOM	1053	CZ2	TRP	A	516	13.015	6.160	9.569	1.00	3.24	C
ATOM	1054	C	TRP	A	516	17.952	5.169	12.003	1.00	4.43	C
ATOM	1055	O	TRP	A	516	17.926	6.353	11.702	1.00	3.37	O
ATOM	1056	N	ILE	A	517	17.666	4.740	13.200	1.00	3.57	N
ATOM	1057	CA	ILE	A	517	17.185	5.585	14.267	1.00	4.13	C
ATOM	1058	CB	ILE	A	517	16.858	4.736	15.545	1.00	3.53	C

ATOM	1059	CG1	ILE	A	517	15.951	5.447	16.492	1.00	3.79	C
ATOM	1060	CD1	ILE	A	517	14.834	6.161	15.859	1.00	2.00	C
ATOM	1061	CG2	ILE	A	517	18.075	4.328	16.251	1.00	2.00	C
ATOM	1062	C	ILE	A	517	18.212	6.609	14.585	1.00	6.38	C
ATOM	1063	O	ILE	A	517	17.848	7.674	15.015	1.00	8.32	O
ATOM	1064	N	LEU	A	518	19.497	6.317	14.379	1.00	7.30	N
ATOM	1065	CA	LEU	A	518	20.514	7.275	14.739	1.00	6.90	C
ATOM	1066	CB	LEU	A	518	21.899	6.677	14.639	1.00	7.32	C
ATOM	1067	CG	LEU	A	518	22.196	5.522	15.627	1.00	8.35	C
ATOM	1068	CD1	LEU	A	518	23.684	5.126	15.647	1.00	2.50	C
ATOM	1069	CD2	LEU	A	518	21.682	5.833	16.977	1.00	5.08	C
ATOM	1070	C	LEU	A	518	20.392	8.434	13.817	1.00	7.74	C
ATOM	1071	O	LEU	A	518	20.237	9.526	14.269	1.00	7.58	O
ATOM	1072	N	ASN	A	519	20.409	8.196	12.511	1.00	9.38	N
ATOM	1073	CA	ASN	A	519	20.366	9.250	11.525	1.00	11.13	C
ATOM	1074	CB	ASN	A	519	20.446	8.593	10.162	1.00	13.71	C
ATOM	1075	CG	ASN	A	519	21.098	9.498	9.094	1.00	23.00	C
ATOM	1076	OD1	ASN	A	519	22.350	9.727	9.100	1.00	30.67	O
ATOM	1077	ND2	ASN	A	519	20.268	10.018	8.169	1.00	22.67	N
ATOM	1078	C	ASN	A	519	19.046	10.037	11.701	1.00	10.46	C
ATOM	1079	O	ASN	A	519	19.004	11.240	11.786	1.00	11.31	O
ATOM	1080	N	VAL	A	520	17.949	9.344	11.879	1.00	9.13	N
ATOM	1081	CA	VAL	A	520	16.709	10.025	12.095	1.00	8.53	C
ATOM	1082	CB	VAL	A	520	15.620	8.949	12.461	1.00	10.43	C
ATOM	1083	CG1	VAL	A	520	14.333	9.580	12.952	1.00	10.55	C
ATOM	1084	CG2	VAL	A	520	15.317	8.122	11.201	1.00	13.73	C
ATOM	1085	C	VAL	A	520	16.771	11.115	13.191	1.00	6.90	C
ATOM	1086	O	VAL	A	520	16.164	12.190	13.044	1.00	3.70	O
ATOM	1087	N	LEU	A	521	17.443	10.792	14.314	1.00	5.11	N
ATOM	1088	CA	LEU	A	521	17.522	11.711	15.441	1.00	4.30	C
ATOM	1089	CB	LEU	A	521	17.357	10.946	16.736	1.00	4.31	C
ATOM	1090	CG	LEU	A	521	16.071	10.118	16.854	1.00	7.22	C
ATOM	1091	CD1	LEU	A	521	15.983	9.289	18.178	1.00	7.33	C
ATOM	1092	CD2	LEU	A	521	14.901	11.002	16.779	1.00	7.22	C
ATOM	1093	C	LEU	A	521	18.823	12.577	15.474	1.00	4.02	C
ATOM	1094	O	LEU	A	521	19.011	13.401	16.394	1.00	2.26	O
ATOM	1095	N	ASN	A	522	19.688	12.407	14.458	1.00	2.73	N
ATOM	1096	CA	ASN	A	522	20.955	13.075	14.488	1.00	2.77	C

ATOM	1097	CB	ASN	A	522	20.752	14.599	14.324	1.00	3.11	C
ATOM	1098	CG	ASN	A	522	21.989	15.287	13.874	1.00	2.00	C
ATOM	1099	OD1	ASN	A	522	22.890	14.661	13.307	1.00	5.97	O
ATOM	1100	ND2	ASN	A	522	22.010	16.571	13.998	1.00	2.15	N
ATOM	1101	C	ASN	A	522	21.802	12.771	15.773	1.00	2.00	C
ATOM	1102	O	ASN	A	522	22.511	13.624	16.287	1.00	3.48	O
ATOM	1103	N	LEU	A	523	21.783	11.539	16.200	1.00	2.26	N
ATOM	1104	CA	LEU	A	523	22.438	11.082	17.427	1.00	3.51	C
ATOM	1105	CB	LEU	A	523	21.428	10.220	18.177	1.00	2.69	C
ATOM	1106	CG	LEU	A	523	21.532	9.986	19.629	1.00	3.52	C
ATOM	1107	CD1	LEU	A	523	20.849	8.528	19.873	1.00	3.71	C
ATOM	1108	CD2	LEU	A	523	22.971	9.957	19.828	1.00	12.53	C
ATOM	1109	C	LEU	A	523	23.614	10.191	17.090	1.00	3.88	C
ATOM	1110	O	LEU	A	523	23.485	9.219	16.297	1.00	4.01	O
ATOM	1111	N	LYS	A	524	24.746	10.461	17.716	1.00	2.74	N
ATOM	1112	CA	LYS	A	524	25.903	9.601	17.474	1.00	2.84	C
ATOM	1113	CB	LYS	A	524	27.149	10.334	17.836	1.00	2.00	C
ATOM	1114	CG	LYS	A	524	27.149	11.724	17.147	1.00	2.00	C
ATOM	1115	CD	LYS	A	524	27.457	11.584	15.679	1.00	2.78	C
ATOM	1116	CE	LYS	A	524	27.418	12.949	14.980	1.00	7.61	C
ATOM	1117	NZ	LYS	A	524	27.359	12.847	13.479	1.00	11.33	N
ATOM	1118	C	LYS	A	524	25.885	8.202	18.109	1.00	3.34	C
ATOM	1119	O	LYS	A	524	25.280	7.964	19.167	1.00	3.82	O
ATOM	1120	N	ALA	A	525	26.506	7.261	17.441	1.00	3.11	N
ATOM	1121	CA	ALA	A	525	26.598	5.910	17.958	1.00	3.88	C
ATOM	1122	CB	ALA	A	525	27.316	5.015	16.961	1.00	2.69	C
ATOM	1123	C	ALA	A	525	27.273	5.816	19.369	1.00	5.48	C
ATOM	1124	O	ALA	A	525	26.858	5.010	20.264	1.00	5.29	O
ATOM	1125	N	PHE	A	526	28.325	6.610	19.571	1.00	5.00	N
ATOM	1126	CA	PHE	A	526	29.027	6.484	20.806	1.00	5.18	C
ATOM	1127	CB	PHE	A	526	30.353	7.286	20.777	1.00	5.32	C
ATOM	1128	CG	PHE	A	526	31.143	7.206	22.059	1.00	6.17	C
ATOM	1129	CD1	PHE	A	526	31.814	6.036	22.377	1.00	2.97	C
ATOM	1130	CE1	PHE	A	526	32.505	5.936	23.581	1.00	3.73	C
ATOM	1131	CZ	PHE	A	526	32.494	7.010	24.568	1.00	2.63	C
ATOM	1132	CE2	PHE	A	526	31.822	8.187	24.280	1.00	3.05	C
ATOM	1133	CD2	PHE	A	526	31.111	8.274	23.014	1.00	5.63	C
ATOM	1134	C	PHE	A	526	28.109	6.884	21.983	1.00	5.59	C

ATOM	1135	O	PHE	A	526	28.240	6.292	23.098	1.00	4.24	O
ATOM	1136	N	ASP	A	527	27.251	7.911	21.773	1.00	4.53	N
ATOM	1137	CA	ASP	A	527	26.313	8.356	22.846	1.00	4.18	C
ATOM	1138	CB	ASP	A	527	25.701	9.662	22.496	1.00	3.20	C
ATOM	1139	CG	ASP	A	527	26.718	10.775	22.359	1.00	5.73	C
ATOM	1140	OD1	ASP	A	527	27.665	10.941	23.205	1.00	6.84	O
ATOM	1141	OD2	ASP	A	527	26.598	11.619	21.454	1.00	9.35	O
ATOM	1142	C	ASP	A	527	25.187	7.375	23.150	1.00	4.67	C
ATOM	1143	O	ASP	A	527	24.739	7.280	24.286	1.00	6.22	O
ATOM	1144	N	PHE	A	528	24.737	6.649	22.136	1.00	4.38	N
ATOM	1145	CA	PHE	A	528	23.658	5.687	22.227	1.00	6.14	C
ATOM	1146	CB	PHE	A	528	23.358	5.130	20.803	1.00	7.25	C
ATOM	1147	CG	PHE	A	528	22.132	4.250	20.713	1.00	8.05	C
ATOM	1148	CD1	PHE	A	528	20.924	4.782	20.311	1.00	6.37	C
ATOM	1149	CE1	PHE	A	528	19.799	3.975	20.164	1.00	7.19	C
ATOM	1150	CZ	PHE	A	528	19.874	2.577	20.441	1.00	5.82	C
ATOM	1151	CE2	PHE	A	528	21.068	2.038	20.784	1.00	5.09	C
ATOM	1152	CD2	PHE	A	528	22.218	2.866	20.917	1.00	7.19	C
ATOM	1153	C	PHE	A	528	24.105	4.578	23.126	1.00	6.06	C
ATOM	1154	O	PHE	A	528	23.425	4.228	24.084	1.00	6.25	O
ATOM	1155	N	TYR	A	529	25.289	4.066	22.816	1.00	6.43	N
ATOM	1156	CA	TYR	A	529	25.938	3.007	23.562	1.00	6.94	C
ATOM	1157	CB	TYR	A	529	27.387	2.762	23.011	1.00	7.10	C
ATOM	1158	CG	TYR	A	529	28.385	2.752	24.090	1.00	7.19	C
ATOM	1159	CD1	TYR	A	529	28.491	1.668	24.986	1.00	11.52	C
ATOM	1160	CE1	TYR	A	529	29.389	1.711	26.088	1.00	10.35	C
ATOM	1161	CZ	TYR	A	529	30.151	2.858	26.287	1.00	13.78	C
ATOM	1162	OH	TYR	A	529	31.044	2.977	27.345	1.00	19.36	O
ATOM	1163	CE2	TYR	A	529	30.068	3.915	25.405	1.00	11.15	C
ATOM	1164	CD2	TYR	A	529	29.151	3.849	24.312	1.00	8.73	C
ATOM	1165	C	TYR	A	529	25.935	3.312	25.069	1.00	7.03	C
ATOM	1166	O	TYR	A	529	25.690	2.457	25.848	1.00	6.96	O
ATOM	1167	N	LYS	A	530	26.238	4.532	25.478	1.00	7.01	N
ATOM	1168	CA	LYS	A	530	26.239	4.848	26.893	1.00	7.93	C
ATOM	1169	CB	LYS	A	530	26.554	6.323	27.075	1.00	8.59	C
ATOM	1170	CG	LYS	A	530	27.919	6.736	26.434	1.00	12.70	C
ATOM	1171	CD	LYS	A	530	28.593	7.898	27.168	1.00	15.96	C
ATOM	1172	CE	LYS	A	530	27.983	9.237	26.949	1.00	16.66	C

ATOM	1173	NZ	LYS	A	530	28.524	10.243	27.977	1.00	21.28	N
ATOM	1174	C	LYS	A	530	24.930	4.531	27.635	1.00	7.04	C
ATOM	1175	O	LYS	A	530	24.894	4.454	28.847	1.00	6.48	O
ATOM	1176	N	VAL	A	531	23.871	4.272	26.892	1.00	6.56	N
ATOM	1177	CA	VAL	A	531	22.577	4.052	27.500	1.00	6.44	C
ATOM	1178	CB	VAL	A	531	21.516	4.971	26.840	1.00	7.07	C
ATOM	1179	CG1	VAL	A	531	20.343	4.227	26.381	1.00	6.11	C
ATOM	1180	CG2	VAL	A	531	21.123	6.035	27.787	1.00	5.82	C
ATOM	1181	C	VAL	A	531	22.123	2.598	27.510	1.00	6.24	C
ATOM	1182	O	VAL	A	531	21.231	2.236	28.299	1.00	5.96	O
ATOM	1183	N	ILE	A	532	22.781	1.762	26.700	1.00	5.58	N
ATOM	1184	CA	ILE	A	532	22.429	0.353	26.549	1.00	5.19	C
ATOM	1185	CB	ILE	A	532	23.238	-0.250	25.456	1.00	4.47	C
ATOM	1186	CG1	ILE	A	532	22.889	0.411	24.083	1.00	4.56	C
ATOM	1187	CD1	ILE	A	532	23.696	-0.133	22.877	1.00	2.00	C
ATOM	1188	CG2	ILE	A	532	22.953	-1.674	25.387	1.00	4.32	C
ATOM	1189	C	ILE	A	532	22.488	-0.511	27.837	1.00	6.67	C
ATOM	1190	O	ILE	A	532	21.454	-1.055	28.285	1.00	7.52	O
ATOM	1191	N	GLU	A	533	23.629	-0.609	28.507	1.00	6.39	N
ATOM	1192	CA	GLU	A	533	23.677	-1.499	29.691	1.00	6.52	C
ATOM	1193	CB	GLU	A	533	25.067	-1.550	30.317	1.00	6.68	C
ATOM	1194	CG	GLU	A	533	25.272	-2.671	31.320	1.00	11.17	C
ATOM	1195	CD	GLU	A	533	26.738	-2.845	31.725	1.00	16.80	C
ATOM	1196	OE1	GLU	A	533	27.562	-2.996	30.800	1.00	19.44	O
ATOM	1197	OE2	GLU	A	533	27.094	-2.828	32.935	1.00	16.76	O
ATOM	1198	C	GLU	A	533	22.683	-1.098	30.776	1.00	6.18	C
ATOM	1199	O	GLU	A	533	22.077	-1.966	31.395	1.00	6.74	O
ATOM	1200	N	SER	A	534	22.497	0.211	30.998	1.00	5.64	N
ATOM	1201	CA	SER	A	534	21.585	0.679	32.030	1.00	4.84	C
ATOM	1202	CB	SER	A	534	21.769	2.187	32.279	1.00	4.45	C
ATOM	1203	OG	SER	A	534	23.070	2.400	32.781	1.00	5.10	O
ATOM	1204	C	SER	A	534	20.139	0.394	31.664	1.00	5.13	C
ATOM	1205	O	SER	A	534	19.329	0.055	32.511	1.00	4.57	O
ATOM	1206	N	PHE	A	535	19.828	0.544	30.377	1.00	5.26	N
ATOM	1207	CA	PHE	A	535	18.497	0.293	29.885	1.00	4.73	C
ATOM	1208	CB	PHE	A	535	18.453	0.649	28.394	1.00	4.00	C
ATOM	1209	CG	PHE	A	535	17.077	0.596	27.794	1.00	5.70	C
ATOM	1210	CD1	PHE	A	535	16.418	-0.623	27.601	1.00	6.27	C

ATOM	1211	CE1	PHE	A	535	15.157	-0.682	27.055	1.00	4.58	C
ATOM	1212	CZ	PHE	A	535	14.532	0.449	26.709	1.00	4.63	C
ATOM	1213	CE2	PHE	A	535	15.156	1.683	26.907	1.00	7.49	C
ATOM	1214	CD2	PHE	A	535	16.430	1.759	27.424	1.00	6.81	C
ATOM	1215	C	PHE	A	535	18.138	-1.186	30.165	1.00	4.51	C
ATOM	1216	O	PHE	A	535	17.052	-1.477	30.621	1.00	3.71	O
ATOM	1217	N	ILE	A	536	19.077	-2.093	29.898	1.00	4.10	N
ATOM	1218	CA	ILE	A	536	18.874	-3.495	30.168	1.00	4.80	C
ATOM	1219	CB	ILE	A	536	20.025	-4.347	29.670	1.00	4.93	C
ATOM	1220	CG1	ILE	A	536	20.014	-4.414	28.161	1.00	2.00	C
ATOM	1221	CD1	ILE	A	536	21.367	-4.726	27.637	1.00	2.00	C
ATOM	1222	CG2	ILE	A	536	19.894	-5.757	30.160	1.00	2.46	C
ATOM	1223	C	ILE	A	536	18.664	-3.836	31.638	1.00	6.22	C
ATOM	1224	O	ILE	A	536	17.956	-4.791	31.910	1.00	7.20	O
ATOM	1225	N	LYS	A	537	19.245	-3.082	32.571	1.00	7.13	N
ATOM	1226	CA	LYS	A	537	19.039	-3.360	34.010	1.00	7.81	C
ATOM	1227	CB	LYS	A	537	20.210	-2.954	34.920	1.00	8.38	C
ATOM	1228	CG	LYS	A	537	21.589	-3.503	34.638	1.00	11.82	C
ATOM	1229	CD	LYS	A	537	22.582	-2.777	35.588	1.00	20.54	C
ATOM	1230	CE	LYS	A	537	24.072	-2.945	35.157	1.00	26.43	C
ATOM	1231	NZ	LYS	A	537	25.029	-2.886	36.319	1.00	26.23	N
ATOM	1232	C	LYS	A	537	17.853	-2.665	34.540	1.00	6.91	C
ATOM	1233	O	LYS	A	537	17.360	-3.015	35.570	1.00	7.82	O
ATOM	1234	N	ALA	A	538	17.402	-1.626	33.873	1.00	6.92	N
ATOM	1235	CA	ALA	A	538	16.250	-0.901	34.370	1.00	5.49	C
ATOM	1236	CB	ALA	A	538	16.297	0.503	33.897	1.00	4.12	C
ATOM	1237	C	ALA	A	538	14.926	-1.537	33.966	1.00	6.38	C
ATOM	1238	O	ALA	A	538	13.957	-1.305	34.626	1.00	6.33	O
ATOM	1239	N	GLU	A	539	14.879	-2.296	32.870	1.00	7.70	N
ATOM	1240	CA	GLU	A	539	13.655	-2.885	32.354	1.00	8.69	C
ATOM	1241	CB	GLU	A	539	13.550	-2.681	30.821	1.00	10.15	C
ATOM	1242	CG	GLU	A	539	12.180	-3.034	30.261	1.00	10.13	C
ATOM	1243	CD	GLU	A	539	11.089	-2.643	31.275	1.00	14.92	C
ATOM	1244	OE1	GLU	A	539	10.984	-1.404	31.629	1.00	14.92	O
ATOM	1245	OE2	GLU	A	539	10.377	-3.560	31.747	1.00	11.46	O
ATOM	1246	C	GLU	A	539	13.662	-4.373	32.559	1.00	9.87	C
ATOM	1247	O	GLU	A	539	14.241	-5.145	31.725	1.00	11.40	O
ATOM	1248	N	GLY	A	540	12.982	-4.820	33.599	1.00	8.74	N

ATOM	1249	CA	GLY	A	540	12.926	-6.240	33.832	1.00	8.45	C
ATOM	1250	C	GLY	A	540	12.031	-7.044	32.889	1.00	8.50	C
ATOM	1251	O	GLY	A	540	12.013	-8.249	32.981	1.00	8.50	O
ATOM	1252	N	ASN	A	541	11.296	-6.412	31.987	1.00	8.51	N
ATOM	1253	CA	ASN	A	541	10.420	-7.177	31.125	1.00	9.67	C
ATOM	1254	CB	ASN	A	541	9.033	-6.558	31.090	1.00	9.96	C
ATOM	1255	CG	ASN	A	541	8.315	-6.684	32.421	1.00	12.87	C
ATOM	1256	OD1	ASN	A	541	7.510	-7.576	32.607	1.00	15.20	O
ATOM	1257	ND2	ASN	A	541	8.603	-5.782	33.346	1.00	11.13	N
ATOM	1258	C	ASN	A	541	10.911	-7.378	29.706	1.00	9.56	C
ATOM	1259	O	ASN	A	541	10.126	-7.663	28.823	1.00	10.01	O
ATOM	1260	N	LEU	A	542	12.207	-7.232	29.472	1.00	9.76	N
ATOM	1261	CA	LEU	A	542	12.717	-7.373	28.095	1.00	9.10	C
ATOM	1262	CB	LEU	A	542	14.075	-6.684	27.941	1.00	8.09	C
ATOM	1263	CG	LEU	A	542	14.095	-5.179	27.973	1.00	8.97	C
ATOM	1264	CD1	LEU	A	542	15.492	-4.668	28.053	1.00	9.22	C
ATOM	1265	CD2	LEU	A	542	13.403	-4.622	26.759	1.00	9.80	C
ATOM	1266	C	LEU	A	542	12.852	-8.848	27.746	1.00	8.30	C
ATOM	1267	O	LEU	A	542	13.338	-9.615	28.540	1.00	8.47	O
ATOM	1268	N	THR	A	543	12.463	-9.247	26.547	1.00	8.14	N
ATOM	1269	CA	THR	A	543	12.631	-10.650	26.147	1.00	7.80	C
ATOM	1270	CB	THR	A	543	11.922	-10.978	24.831	1.00	6.70	C
ATOM	1271	OG1	THR	A	543	12.469	-10.196	23.781	1.00	4.89	O
ATOM	1272	CG2	THR	A	543	10.487	-10.605	24.853	1.00	7.19	C
ATOM	1273	C	THR	A	543	14.089	-11.004	25.939	1.00	9.04	C
ATOM	1274	O	THR	A	543	14.967	-10.139	25.938	1.00	9.69	O
ATOM	1275	N	ARG	A	544	14.325	-12.283	25.690	1.00	9.66	N
ATOM	1276	CA	ARG	A	544	15.657	-12.785	25.472	1.00	10.93	C
ATOM	1277	CB	ARG	A	544	15.645	-14.329	25.540	1.00	11.59	C
ATOM	1278	CG	ARG	A	544	16.929	-15.067	25.014	1.00	10.88	C
ATOM	1279	CD	ARG	A	544	16.848	-16.618	25.167	1.00	14.78	C
ATOM	1280	NE	ARG	A	544	15.749	-17.233	24.413	1.00	13.02	N
ATOM	1281	CZ	ARG	A	544	15.747	-17.391	23.074	1.00	18.91	C
ATOM	1282	NH1	ARG	A	544	16.775	-16.942	22.355	1.00	23.09	N
ATOM	1283	NH2	ARG	A	544	14.719	-17.965	22.422	1.00	17.48	N
ATOM	1284	C	ARG	A	544	16.117	-12.289	24.106	1.00	11.05	C
ATOM	1285	O	ARG	A	544	17.262	-11.979	23.932	1.00	10.33	O
ATOM	1286	N	GLU	A	545	15.186	-12.211	23.167	1.00	11.63	N

ATOM	1287	CA	GLU	A	545	15.455	-11.772	21.819	1.00	13.95	C
ATOM	1288	CB	GLU	A	545	14.246	-12.016	20.946	1.00	13.76	C
ATOM	1289	CG	GLU	A	545	13.860	-13.495	20.890	1.00	21.85	C
ATOM	1290	CD	GLU	A	545	13.715	-14.208	22.292	1.00	28.21	C
ATOM	1291	OE1	GLU	A	545	13.028	-13.699	23.251	1.00	22.99	O
ATOM	1292	OE2	GLU	A	545	14.307	-15.320	22.427	1.00	29.40	O
ATOM	1293	C	GLU	A	545	15.772	-10.298	21.757	1.00	14.02	C
ATOM	1294	O	GLU	A	545	16.548	-9.871	20.921	1.00	14.84	O
ATOM	1295	N	MET	A	546	15.154	-9.530	22.646	1.00	13.93	N
ATOM	1296	CA	MET	A	546	15.330	-8.086	22.725	1.00	13.00	C
ATOM	1297	CB	MET	A	546	14.159	-7.478	23.524	1.00	13.31	C
ATOM	1298	CG	MET	A	546	13.948	-5.997	23.287	1.00	19.54	C
ATOM	1299	SD	MET	A	546	13.855	-5.454	21.439	1.00	29.26	S
ATOM	1300	CE	MET	A	546	15.547	-5.068	21.117	1.00	21.36	C
ATOM	1301	C	MET	A	546	16.706	-7.727	23.314	1.00	10.12	C
ATOM	1302	O	MET	A	546	17.354	-6.831	22.867	1.00	7.74	O
ATOM	1303	N	ILE	A	547	17.154	-8.475	24.313	1.00	9.83	N
ATOM	1304	CA	ILE	A	547	18.459	-8.235	24.923	1.00	8.79	C
ATOM	1305	CB	ILE	A	547	18.601	-9.080	26.159	1.00	7.97	C
ATOM	1306	CG1	ILE	A	547	17.582	-8.632	27.190	1.00	7.88	C
ATOM	1307	CD1	ILE	A	547	17.608	-9.481	28.521	1.00	7.89	C
ATOM	1308	CG2	ILE	A	547	19.986	-8.952	26.827	1.00	8.85	C
ATOM	1309	C	ILE	A	547	19.476	-8.603	23.875	1.00	8.59	C
ATOM	1310	O	ILE	A	547	20.432	-7.911	23.585	1.00	9.01	O
ATOM	1311	N	LYS	A	548	19.203	-9.683	23.224	1.00	8.48	N
ATOM	1312	CA	LYS	A	548	20.060	-10.106	22.157	1.00	8.58	C
ATOM	1313	CB	LYS	A	548	19.527	-11.417	21.580	1.00	8.46	C
ATOM	1314	CG	LYS	A	548	20.646	-12.366	21.115	1.00	14.13	C
ATOM	1315	CD	LYS	A	548	20.837	-13.592	22.053	1.00	20.90	C
ATOM	1316	CE	LYS	A	548	21.254	-13.189	23.487	1.00	24.85	C
ATOM	1317	NZ	LYS	A	548	21.477	-14.338	24.469	1.00	25.80	N
ATOM	1318	C	LYS	A	548	20.211	-9.024	21.088	1.00	7.39	C
ATOM	1319	O	LYS	A	548	21.321	-8.759	20.627	1.00	7.65	O
ATOM	1320	N	HIS	A	549	19.100	-8.402	20.689	1.00	5.99	N
ATOM	1321	CA	HIS	A	549	19.118	-7.426	19.629	1.00	3.72	C
ATOM	1322	CB	HIS	A	549	17.703	-7.050	19.213	1.00	2.50	C
ATOM	1323	CG	HIS	A	549	17.656	-5.973	18.172	1.00	4.11	C
ATOM	1324	ND1	HIS	A	549	18.258	-6.102	16.932	1.00	2.57	N

ATOM	1325	CE1	HIS	A	549	18.083	-4.979	16.253	1.00	2.00	C
ATOM	1326	NE2	HIS	A	549	17.394	-4.134	17.003	1.00	2.00	N
ATOM	1327	CD2	HIS	A	549	17.121	-4.725	18.206	1.00	2.00	C
ATOM	1328	C	HIS	A	549	19.919	-6.219	20.099	1.00	4.21	C
ATOM	1329	O	HIS	A	549	20.773	-5.673	19.357	1.00	2.85	O
ATOM	1330	N	LEU	A	550	19.698	-5.856	21.366	1.00	4.44	N
ATOM	1331	CA	LEU	A	550	20.395	-4.711	21.962	1.00	5.58	C
ATOM	1332	CB	LEU	A	550	19.851	-4.379	23.369	1.00	4.96	C
ATOM	1333	CG	LEU	A	550	18.486	-3.698	23.396	1.00	6.21	C
ATOM	1334	CD1	LEU	A	550	18.194	-3.255	24.820	1.00	9.90	C
ATOM	1335	CD2	LEU	A	550	18.512	-2.473	22.485	1.00	8.87	C
ATOM	1336	C	LEU	A	550	21.912	-4.937	21.991	1.00	5.86	C
ATOM	1337	O	LEU	A	550	22.693	-4.018	21.757	1.00	5.64	O
ATOM	1338	N	GLU	A	551	22.318	-6.167	22.289	1.00	5.89	N
ATOM	1339	CA	GLU	A	551	23.714	-6.493	22.297	1.00	7.35	C
ATOM	1340	CB	GLU	A	551	23.897	-7.847	22.907	1.00	7.43	C
ATOM	1341	CG	GLU	A	551	25.312	-8.358	22.922	1.00	11.11	C
ATOM	1342	CD	GLU	A	551	25.376	-9.858	23.196	1.00	12.97	C
ATOM	1343	OE1	GLU	A	551	25.783	-10.217	24.325	1.00	13.82	O
ATOM	1344	OE2	GLU	A	551	25.015	-10.655	22.287	1.00	12.23	O
ATOM	1345	C	GLU	A	551	24.347	-6.418	20.897	1.00	7.94	C
ATOM	1346	O	GLU	A	551	25.475	-5.935	20.720	1.00	8.12	O
ATOM	1347	N	ARG	A	552	23.616	-6.849	19.888	1.00	8.62	N
ATOM	1348	CA	ARG	A	552	24.128	-6.750	18.529	1.00	10.18	C
ATOM	1349	CB	ARG	A	552	23.144	-7.403	17.595	1.00	12.41	C
ATOM	1350	CG	ARG	A	552	23.649	-7.583	16.190	1.00	20.85	C
ATOM	1351	CD	ARG	A	552	24.954	-8.372	16.069	1.00	27.00	C
ATOM	1352	NE	ARG	A	552	25.734	-7.818	14.969	1.00	30.08	N
ATOM	1353	CZ	ARG	A	552	27.060	-7.851	14.950	1.00	34.49	C
ATOM	1354	NH1	ARG	A	552	27.664	-8.435	15.999	1.00	30.27	N
ATOM	1355	NH2	ARG	A	552	27.773	-7.319	13.901	1.00	34.69	N
ATOM	1356	C	ARG	A	552	24.352	-5.292	18.076	1.00	9.36	C
ATOM	1357	O	ARG	A	552	25.304	-5.020	17.357	1.00	9.30	O
ATOM	1358	N	CYS	A	553	23.467	-4.381	18.496	1.00	7.47	N
ATOM	1359	CA	CYS	A	553	23.615	-2.972	18.243	1.00	7.51	C
ATOM	1360	CB	CYS	A	553	22.387	-2.146	18.736	1.00	7.23	C
ATOM	1361	SG	CYS	A	553	20.754	-2.427	17.964	1.00	7.13	S
ATOM	1362	C	CYS	A	553	24.890	-2.480	18.971	1.00	7.59	C

ATOM	1363	O	CYS	A	553	25.704	-1.706	18.435	1.00	7.17	O
ATOM	1364	N	GLU	A	554	25.084	-2.959	20.180	1.00	6.68	N
ATOM	1365	CA	GLU	A	554	26.265	-2.557	20.905	1.00	8.06	C
ATOM	1366	CB	GLU	A	554	26.211	-3.111	22.321	1.00	7.22	C
ATOM	1367	CG	GLU	A	554	27.140	-2.424	23.280	1.00	5.98	C
ATOM	1368	CD	GLU	A	554	26.917	-2.886	24.688	1.00	11.28	C
ATOM	1369	OE1	GLU	A	554	26.704	-4.112	24.903	1.00	15.10	O
ATOM	1370	OE2	GLU	A	554	26.930	-2.034	25.602	1.00	14.58	O
ATOM	1371	C	GLU	A	554	27.576	-2.999	20.274	1.00	8.25	C
ATOM	1372	O	GLU	A	554	28.592	-2.329	20.318	1.00	9.11	O
ATOM	1373	N	HIS	A	555	27.561	-4.184	19.737	1.00	8.65	N
ATOM	1374	CA	HIS	A	555	28.736	-4.736	19.112	1.00	7.90	C
ATOM	1375	CB	HIS	A	555	28.487	-6.229	18.855	1.00	6.62	C
ATOM	1376	CG	HIS	A	555	28.603	-7.083	20.083	1.00	4.39	C
ATOM	1377	ND1	HIS	A	555	28.242	-8.418	20.099	1.00	2.00	N
ATOM	1378	CE1	HIS	A	555	28.523	-8.929	21.283	1.00	2.00	C
ATOM	1379	NE2	HIS	A	555	29.024	-7.971	22.050	1.00	2.00	N
ATOM	1380	CD2	HIS	A	555	29.094	-6.808	21.319	1.00	2.05	C
ATOM	1381	C	HIS	A	555	29.067	-3.985	17.817	1.00	8.31	C
ATOM	1382	O	HIS	A	555	30.235	-3.850	17.416	1.00	8.87	O
ATOM	1383	N	ARG	A	556	28.046	-3.483	17.145	1.00	7.61	N
ATOM	1384	CA	ARG	A	556	28.312	-2.784	15.910	1.00	7.11	C
ATOM	1385	CB	ARG	A	556	27.068	-2.745	15.032	1.00	7.58	C
ATOM	1386	CG	ARG	A	556	26.830	-4.086	14.419	1.00	12.81	C
ATOM	1387	CD	ARG	A	556	25.422	-4.476	14.251	1.00	19.23	C
ATOM	1388	NE	ARG	A	556	24.910	-3.879	13.043	1.00	22.82	N
ATOM	1389	CZ	ARG	A	556	23.632	-3.796	12.766	1.00	25.22	C
ATOM	1390	NH1	ARG	A	556	22.735	-4.276	13.647	1.00	23.17	N
ATOM	1391	NH2	ARG	A	556	23.255	-3.226	11.619	1.00	23.51	N
ATOM	1392	C	ARG	A	556	28.790	-1.417	16.218	1.00	5.89	C
ATOM	1393	O	ARG	A	556	29.447	-0.835	15.400	1.00	6.78	O
ATOM	1394	N	ILE	A	557	28.480	-0.890	17.404	1.00	4.95	N
ATOM	1395	CA	ILE	A	557	28.975	0.438	17.777	1.00	3.96	C
ATOM	1396	CB	ILE	A	557	28.195	0.966	18.957	1.00	4.35	C
ATOM	1397	CG1	ILE	A	557	26.718	1.166	18.578	1.00	3.64	C
ATOM	1398	CD1	ILE	A	557	25.860	1.516	19.797	1.00	2.00	C
ATOM	1399	CG2	ILE	A	557	28.762	2.324	19.538	1.00	2.19	C
ATOM	1400	C	ILE	A	557	30.462	0.279	18.067	1.00	5.06	C

ATOM	1401	O	ILE	A	557	31.301	1.023	17.582	1.00	3.84	O
ATOM	1402	N	MET	A	558	30.774	-0.732	18.862	1.00	6.34	N
ATOM	1403	CA	MET	A	558	32.137	-1.072	19.214	1.00	7.02	C
ATOM	1404	CB	MET	A	558	32.147	-2.170	20.277	1.00	7.34	C
ATOM	1405	CG	MET	A	558	31.501	-1.673	21.619	1.00	12.35	C
ATOM	1406	SD	MET	A	558	31.502	-2.949	22.900	1.00	17.81	S
ATOM	1407	CE	MET	A	558	30.101	-3.923	22.556	1.00	14.43	C
ATOM	1408	C	MET	A	558	33.009	-1.491	18.054	1.00	5.34	C
ATOM	1409	O	MET	A	558	34.222	-1.284	18.091	1.00	4.60	O
ATOM	1410	N	GLU	A	559	32.417	-2.102	17.040	1.00	3.43	N
ATOM	1411	CA	GLU	A	559	33.269	-2.609	15.983	1.00	2.79	C
ATOM	1412	CB	GLU	A	559	32.673	-3.807	15.250	1.00	3.49	C
ATOM	1413	CG	GLU	A	559	31.360	-3.495	14.562	1.00	6.17	C
ATOM	1414	CD	GLU	A	559	30.720	-4.665	13.825	1.00	9.46	C
ATOM	1415	OE1	GLU	A	559	30.780	-5.820	14.299	1.00	6.19	O
ATOM	1416	OE2	GLU	A	559	30.122	-4.376	12.742	1.00	13.37	O
ATOM	1417	C	GLU	A	559	33.642	-1.514	15.017	1.00	2.46	C
ATOM	1418	O	GLU	A	559	34.777	-1.515	14.553	1.00	3.03	O
ATOM	1419	N	SER	A	560	32.722	-0.585	14.708	1.00	2.00	N
ATOM	1420	CA	SER	A	560	32.999	0.509	13.765	1.00	2.00	C
ATOM	1421	CB	SER	A	560	32.848	0.074	12.287	1.00	2.00	C
ATOM	1422	OG	SER	A	560	31.566	-0.370	11.966	1.00	2.00	O
ATOM	1423	C	SER	A	560	32.339	1.845	13.960	1.00	2.00	C
ATOM	1424	O	SER	A	560	33.008	2.816	14.009	1.00	2.06	O
ATOM	1425	N	LEU	A	561	31.020	1.902	14.097	1.00	2.00	N
ATOM	1426	CA	LEU	A	561	30.323	3.156	14.220	1.00	2.20	C
ATOM	1427	CB	LEU	A	561	28.835	2.896	14.518	1.00	2.33	C
ATOM	1428	CG	LEU	A	561	27.969	2.019	13.593	1.00	4.31	C
ATOM	1429	CD1	LEU	A	561	26.528	1.785	14.215	1.00	2.00	C
ATOM	1430	CD2	LEU	A	561	27.927	2.524	12.106	1.00	2.00	C
ATOM	1431	C	LEU	A	561	30.959	4.193	15.219	1.00	2.00	C
ATOM	1432	O	LEU	A	561	31.119	5.361	14.911	1.00	2.00	O
ATOM	1433	N	ALA	A	562	31.326	3.756	16.393	1.00	2.00	N
ATOM	1434	CA	ALA	A	562	31.879	4.693	17.354	1.00	2.83	C
ATOM	1435	CB	ALA	A	562	31.979	4.095	18.810	1.00	2.00	C
ATOM	1436	C	ALA	A	562	33.259	5.109	16.884	1.00	3.11	C
ATOM	1437	O	ALA	A	562	33.863	5.921	17.530	1.00	3.18	O
ATOM	1438	N	TRP	A	563	33.768	4.535	15.806	1.00	2.21	N

ATOM	1439	CA	TRP	A	563	35.073	4.973	15.316	1.00	3.35	C
ATOM	1440	CB	TRP	A	563	36.036	3.777	15.101	1.00	2.70	C
ATOM	1441	CG	TRP	A	563	36.208	2.881	16.308	1.00	3.50	C
ATOM	1442	CD1	TRP	A	563	35.434	1.796	16.638	1.00	4.08	C
ATOM	1443	NE1	TRP	A	563	35.881	1.214	17.793	1.00	2.00	N
ATOM	1444	CE2	TRP	A	563	36.974	1.908	18.231	1.00	2.92	C
ATOM	1445	CD2	TRP	A	563	37.222	2.948	17.292	1.00	2.00	C
ATOM	1446	CE3	TRP	A	563	38.273	3.804	17.524	1.00	2.65	C
ATOM	1447	CZ3	TRP	A	563	39.083	3.601	18.648	1.00	3.77	C
ATOM	1448	CH2	TRP	A	563	38.839	2.532	19.547	1.00	2.00	C
ATOM	1449	CZ2	TRP	A	563	37.786	1.694	19.378	1.00	2.00	C
ATOM	1450	C	TRP	A	563	34.969	5.825	14.016	1.00	3.80	C
ATOM	1451	O	TRP	A	563	35.925	6.044	13.306	1.00	2.92	O
ATOM	1452	N	LEU	A	564	33.777	6.253	13.660	1.00	4.71	N
ATOM	1453	CA	LEU	A	564	33.712	7.145	12.484	1.00	5.58	C
ATOM	1454	CB	LEU	A	564	32.264	7.290	11.965	1.00	4.26	C
ATOM	1455	CG	LEU	A	564	31.566	6.068	11.390	1.00	4.77	C
ATOM	1456	CD1	LEU	A	564	30.004	6.356	11.192	1.00	3.32	C
ATOM	1457	CD2	LEU	A	564	32.200	5.550	10.050	1.00	2.00	C
ATOM	1458	C	LEU	A	564	34.290	8.532	12.858	1.00	4.78	C
ATOM	1459	O	LEU	A	564	34.350	8.918	14.034	1.00	4.33	O
ATOM	1460	N	SER	A	565	34.677	9.272	11.849	1.00	4.86	N
ATOM	1461	CA	SER	A	565	35.281	10.573	12.036	1.00	5.62	C
ATOM	1462	CB	SER	A	565	35.653	11.162	10.720	1.00	6.03	C
ATOM	1463	OG	SER	A	565	36.397	10.281	9.913	1.00	9.07	O
ATOM	1464	C	SER	A	565	34.368	11.553	12.711	1.00	6.16	C
ATOM	1465	O	SER	A	565	34.856	12.519	13.301	1.00	7.64	O
ATOM	1466	N	ASP	A	566	33.058	11.357	12.600	1.00	5.01	N
ATOM	1467	CA	ASP	A	566	32.118	12.194	13.356	1.00	4.61	C
ATOM	1468	CB	ASP	A	566	30.751	12.235	12.667	1.00	4.01	C
ATOM	1469	CG	ASP	A	566	30.043	10.859	12.633	1.00	7.60	C
ATOM	1470	OD1	ASP	A	566	30.719	9.768	12.582	1.00	12.23	O
ATOM	1471	OD2	ASP	A	566	28.798	10.766	12.592	1.00	6.42	O
ATOM	1472	C	ASP	A	566	31.929	11.762	14.835	1.00	4.59	C
ATOM	1473	O	ASP	A	566	31.067	12.257	15.518	1.00	6.37	O
ATOM	1474	N	SER	A	567	32.752	10.892	15.365	1.00	3.80	N
ATOM	1475	CA	SER	A	567	32.472	10.379	16.678	1.00	4.60	C
ATOM	1476	CB	SER	A	567	32.849	8.890	16.709	1.00	4.41	C

ATOM	1477	OG	SER	A	567	32.554	8.341	17.982	1.00	5.48	O
ATOM	1478	C	SER	A	567	33.115	11.092	17.875	1.00	4.42	C
ATOM	1479	O	SER	A	567	34.332	11.220	17.963	1.00	4.31	O
ATOM	1480	N	PRO	A	568	32.300	11.423	18.867	1.00	4.48	N
ATOM	1481	CA	PRO	A	568	32.786	12.087	20.083	1.00	4.54	C
ATOM	1482	CB	PRO	A	568	31.550	12.119	20.963	1.00	4.15	C
ATOM	1483	CG	PRO	A	568	30.425	12.026	20.031	1.00	4.02	C
ATOM	1484	CD	PRO	A	568	30.859	11.141	18.927	1.00	3.92	C
ATOM	1485	C	PRO	A	568	33.922	11.300	20.746	1.00	4.80	C
ATOM	1486	O	PRO	A	568	34.778	11.860	21.382	1.00	5.03	O
ATOM	1487	N	LEU	A	569	33.962	9.997	20.550	1.00	5.56	N
ATOM	1488	CA	LEU	A	569	35.065	9.185	21.063	1.00	5.83	C
ATOM	1489	CB	LEU	A	569	34.953	7.839	20.393	1.00	5.39	C
ATOM	1490	CG	LEU	A	569	35.662	6.643	21.012	1.00	8.02	C
ATOM	1491	CD1	LEU	A	569	36.514	5.968	20.035	1.00	7.12	C
ATOM	1492	CD2	LEU	A	569	36.445	7.041	22.339	1.00	9.13	C
ATOM	1493	C	LEU	A	569	36.523	9.780	20.895	1.00	6.51	C
ATOM	1494	O	LEU	A	569	37.338	9.766	21.816	1.00	7.17	O
ATOM	1495	N	PHE	A	570	36.860	10.317	19.739	1.00	6.86	N
ATOM	1496	CA	PHE	A	570	38.216	10.808	19.528	1.00	7.23	C
ATOM	1497	CB	PHE	A	570	38.501	11.136	18.035	1.00	5.23	C
ATOM	1498	CG	PHE	A	570	38.424	9.923	17.163	1.00	6.73	C
ATOM	1499	CD1	PHE	A	570	39.368	8.914	17.301	1.00	7.09	C
ATOM	1500	CE1	PHE	A	570	39.276	7.757	16.572	1.00	7.82	C
ATOM	1501	CZ	PHE	A	570	38.233	7.573	15.679	1.00	7.51	C
ATOM	1502	CE2	PHE	A	570	37.301	8.556	15.528	1.00	6.38	C
ATOM	1503	CD2	PHE	A	570	37.377	9.719	16.292	1.00	5.05	C
ATOM	1504	C	PHE	A	570	38.524	11.975	20.418	1.00	9.18	C
ATOM	1505	O	PHE	A	570	39.718	12.193	20.765	1.00	10.62	O
ATOM	1506	N	ASP	A	571	37.494	12.747	20.782	1.00	10.38	N
ATOM	1507	CA	ASP	A	571	37.678	13.891	21.705	1.00	12.23	C
ATOM	1508	CB	ASP	A	571	36.503	14.908	21.636	1.00	12.92	C
ATOM	1509	CG	ASP	A	571	36.747	16.079	20.592	1.00	19.58	C
ATOM	1510	OD1	ASP	A	571	35.738	16.784	20.221	1.00	22.58	O
ATOM	1511	OD2	ASP	A	571	37.892	16.388	20.102	1.00	24.68	O
ATOM	1512	C	ASP	A	571	37.838	13.320	23.139	1.00	11.69	C
ATOM	1513	O	ASP	A	571	38.703	13.723	23.898	1.00	9.05	O
ATOM	1514	N	LEU	A	572	37.023	12.322	23.447	1.00	12.36	N

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ATOM   1515  CA  LEU A 572      37.111  11.657  24.705  1.00 14.85           C
ATOM   1516  CB  LEU A 572      36.028  10.621  24.800  1.00 16.18           C
ATOM   1517  CG  LEU A 572      35.809  10.127  26.233  1.00 21.52           C
ATOM   1518  CD1 LEU A 572      35.722  11.348  27.185  1.00 21.46           C
ATOM   1519  CD2 LEU A 572      34.536   9.247  26.291  1.00 23.88           C
ATOM   1520  C   LEU A 572      38.461  10.963  24.850  1.00 15.08           C
ATOM   1521  O   LEU A 572      38.945  10.761  25.954  1.00 15.22           O
ATOM   1522  N   ILE A 573      39.068  10.567  23.745  1.00 15.07           N
ATOM   1523  CA  ILE A 573      40.376   9.968  23.850  1.00 15.55           C
ATOM   1524  CB  ILE A 573      40.645   9.090  22.628  1.00 14.55           C
ATOM   1525  CG1 ILE A 573      39.959   7.746  22.767  1.00 12.31           C
ATOM   1526  CD1 ILE A 573      39.857   6.981  21.393  1.00  6.14           C
ATOM   1527  CG2 ILE A 573      42.098   8.825  22.425  1.00 12.90           C
ATOM   1528  C   ILE A 573      41.435  11.088  23.983  1.00 17.30           C
ATOM   1529  O   ILE A 573      42.414  10.949  24.685  1.00 18.35           O
ATOM   1530  N   LYS A 574      41.261  12.192  23.290  1.00 17.39           N
ATOM   1531  CA  LYS A 574      42.272  13.190  23.373  1.00 18.15           C
ATOM   1532  CB  LYS A 574      42.087  14.242  22.296  1.00 16.97           C
ATOM   1533  CG  LYS A 574      43.280  15.079  22.098  1.00 15.24           C
ATOM   1534  CD  LYS A 574      43.072  16.241  21.114  1.00 15.89           C
ATOM   1535  CE  LYS A 574      44.287  17.213  21.136  1.00 14.11           C
ATOM   1536  NZ  LYS A 574      44.345  18.197  20.020  1.00  9.92           N
ATOM   1537  C   LYS A 574      42.251  13.802  24.760  1.00 20.35           C
ATOM   1538  O   LYS A 574      43.302  13.946  25.401  1.00 20.46           O
ATOM   1539  N   GLN A 575      41.059  14.149  25.224  1.00 22.46           N
ATOM   1540  CA  GLN A 575      40.876  14.743  26.532  1.00 24.95           C
ATOM   1541  CB  GLN A 575      39.394  14.789  26.845  1.00 25.51           C
ATOM   1542  CG  GLN A 575      39.020  15.353  28.210  1.00 31.74           C
ATOM   1543  CD  GLN A 575      37.544  15.802  28.301  1.00 36.07           C
ATOM   1544  OE1 GLN A 575      36.639  14.979  28.181  1.00 37.48           O
ATOM   1545  NE2 GLN A 575      37.315  17.110  28.535  1.00 37.16           N
ATOM   1546  C   GLN A 575      41.569  13.876  27.560  1.00 26.44           C
ATOM   1547  O   GLN A 575      42.042  14.356  28.570  1.00 26.79           O
ATOM   1548  N   SER A 576      41.660  12.579  27.291  1.00 28.20           N
ATOM   1549  CA  SER A 576      42.287  11.655  28.238  1.00 28.79           C
ATOM   1550  CB  SER A 576      41.622  10.312  28.144  1.00 28.17           C
ATOM   1551  OG  SER A 576      42.636   9.371  27.953  1.00 27.25           O
ATOM   1552  C   SER A 576      43.775  11.452  28.024  1.00 29.76           C
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ATOM	1553	O	SER	A	576	44.506	11.186	28.946	1.00	29.92	O
ATOM	1554	N	LYS	A	577	44.210	11.566	26.785	1.00	31.31	N
ATOM	1555	CA	LYS	A	577	45.610	11.424	26.438	1.00	32.44	C
ATOM	1556	CB	LYS	A	577	45.756	11.456	24.924	1.00	32.43	C
ATOM	1557	CG	LYS	A	577	46.759	10.514	24.390	1.00	31.18	C
ATOM	1558	CD	LYS	A	577	46.252	9.097	24.601	1.00	28.82	C
ATOM	1559	CE	LYS	A	577	47.095	8.118	23.806	1.00	29.90	C
ATOM	1560	NZ	LYS	A	577	46.930	6.691	24.174	1.00	25.38	N
ATOM	1561	C	LYS	A	577	46.462	12.556	27.028	1.00	33.67	C
ATOM	1562	O	LYS	A	577	47.676	12.565	26.875	1.00	33.03	O
ATOM	1563	N	ASP	A	578	45.820	13.534	27.663	1.00	35.46	N
ATOM	1564	CA	ASP	A	578	46.552	14.659	28.239	1.00	36.42	C
ATOM	1565	CB	ASP	A	578	45.949	16.006	27.817	1.00	36.95	C
ATOM	1566	CG	ASP	A	578	46.096	16.280	26.331	1.00	38.84	C
ATOM	1567	OD1	ASP	A	578	47.060	15.800	25.685	1.00	41.17	O
ATOM	1568	OD2	ASP	A	578	45.279	16.976	25.708	1.00	42.67	O
ATOM	1569	C	ASP	A	578	46.556	14.554	29.751	1.00	36.86	C
ATOM	1573	N	SER	B	644	36.636	9.547	33.813	1.00	13.34	N
ATOM	1574	CA	SER	B	644	35.896	9.256	32.537	1.00	13.52	C
ATOM	1575	CB	SER	B	644	36.738	9.648	31.317	1.00	14.13	C
ATOM	1576	OG	SER	B	644	35.927	9.799	30.153	1.00	17.99	O
ATOM	1577	C	SER	B	644	35.367	7.811	32.424	1.00	12.17	C
ATOM	1578	O	SER	B	644	35.897	6.982	31.701	1.00	12.64	O
ATOM	1579	N	THR	B	645	34.293	7.546	33.159	1.00	10.72	N
ATOM	1580	CA	THR	B	645	33.630	6.265	33.190	1.00	8.91	C
ATOM	1581	CB	THR	B	645	32.330	6.374	34.033	1.00	9.09	C
ATOM	1582	OG1	THR	B	645	32.625	6.834	35.352	1.00	8.17	O
ATOM	1583	CG2	THR	B	645	31.728	4.968	34.256	1.00	9.39	C
ATOM	1584	C	THR	B	645	33.274	5.785	31.770	1.00	7.52	C
ATOM	1585	O	THR	B	645	33.531	4.625	31.379	1.00	5.65	O
ATOM	1586	N	SER	B	646	32.676	6.694	31.028	1.00	6.11	N
ATOM	1587	CA	SER	B	646	32.310	6.460	29.633	1.00	6.99	C
ATOM	1588	CB	SER	B	646	31.925	7.758	28.930	1.00	7.51	C
ATOM	1589	OG	SER	B	646	32.996	8.717	29.121	1.00	12.87	O
ATOM	1590	C	SER	B	646	33.444	5.841	28.850	1.00	4.97	C
ATOM	1591	O	SER	B	646	33.254	4.809	28.273	1.00	3.36	O
ATOM	1592	N	LEU	B	647	34.606	6.477	28.859	1.00	4.50	N
ATOM	1593	CA	LEU	B	647	35.742	5.969	28.104	1.00	6.01	C

ATOM	1594	CB	LEU	B	647	36.846	6.981	28.058	1.00	6.07	C
ATOM	1595	CG	LEU	B	647	38.046	6.586	27.214	1.00	5.64	C
ATOM	1596	CD1	LEU	B	647	37.711	6.400	25.743	1.00	2.00	C
ATOM	1597	CD2	LEU	B	647	39.120	7.685	27.433	1.00	3.27	C
ATOM	1598	C	LEU	B	647	36.327	4.653	28.634	1.00	7.62	C
ATOM	1599	O	LEU	B	647	36.803	3.822	27.846	1.00	7.75	O
ATOM	1600	N	SER	B	648	36.335	4.459	29.958	1.00	7.31	N
ATOM	1601	CA	SER	B	648	36.813	3.191	30.458	1.00	7.43	C
ATOM	1602	CB	SER	B	648	37.232	3.312	31.940	1.00	8.38	C
ATOM	1603	OG	SER	B	648	36.099	3.311	32.774	1.00	12.14	O
ATOM	1604	C	SER	B	648	35.783	2.054	30.271	1.00	6.33	C
ATOM	1605	O	SER	B	648	36.135	0.897	30.113	1.00	6.45	O
ATOM	1606	N	LEU	B	649	34.499	2.359	30.278	1.00	5.67	N
ATOM	1607	CA	LEU	B	649	33.485	1.304	30.061	1.00	4.38	C
ATOM	1608	CB	LEU	B	649	32.075	1.863	30.294	1.00	3.95	C
ATOM	1609	CG	LEU	B	649	30.936	0.916	30.609	1.00	3.72	C
ATOM	1610	CD1	LEU	B	649	30.121	0.646	29.371	1.00	8.06	C
ATOM	1611	CD2	LEU	B	649	31.444	-0.408	31.175	1.00	2.00	C
ATOM	1612	C	LEU	B	649	33.590	0.812	28.646	1.00	4.70	C
ATOM	1613	O	LEU	B	649	33.553	-0.418	28.356	1.00	6.51	O
ATOM	1614	N	PHE	B	650	33.796	1.774	27.755	1.00	3.18	N
ATOM	1615	CA	PHE	B	650	33.888	1.510	26.366	1.00	2.00	C
ATOM	1616	CB	PHE	B	650	33.940	2.828	25.556	1.00	2.00	C
ATOM	1617	CG	PHE	B	650	33.947	2.604	24.106	1.00	2.00	C
ATOM	1618	CD1	PHE	B	650	32.763	2.357	23.427	1.00	2.00	C
ATOM	1619	CE1	PHE	B	650	32.792	2.111	22.035	1.00	2.00	C
ATOM	1620	CZ	PHE	B	650	33.988	2.062	21.329	1.00	2.00	C
ATOM	1621	CE2	PHE	B	650	35.175	2.284	21.992	1.00	2.00	C
ATOM	1622	CD2	PHE	B	650	35.163	2.543	23.394	1.00	2.00	C
ATOM	1623	C	PHE	B	650	35.103	0.619	26.111	1.00	2.00	C
ATOM	1624	O	PHE	B	650	34.994	-0.415	25.474	1.00	2.37	O
ATOM	1625	N	TYR	B	651	36.266	1.031	26.556	1.00	2.00	N
ATOM	1626	CA	TYR	B	651	37.452	0.270	26.268	1.00	3.35	C
ATOM	1627	CB	TYR	B	651	38.731	0.988	26.767	1.00	3.37	C
ATOM	1628	CG	TYR	B	651	39.419	1.741	25.662	1.00	4.03	C
ATOM	1629	CD1	TYR	B	651	40.287	1.076	24.801	1.00	5.03	C
ATOM	1630	CE1	TYR	B	651	40.882	1.737	23.744	1.00	7.04	C
ATOM	1631	CZ	TYR	B	651	40.633	3.096	23.506	1.00	3.43	C

ATOM	1632	OH	TYR	B	651	41.249	3.679	22.433	1.00	3.35	O
ATOM	1633	CE2	TYR	B	651	39.780	3.780	24.300	1.00	2.37	C
ATOM	1634	CD2	TYR	B	651	39.147	3.087	25.408	1.00	2.56	C
ATOM	1635	C	TYR	B	651	37.335	-1.135	26.856	1.00	4.60	C
ATOM	1636	O	TYR	B	651	37.557	-2.180	26.169	1.00	3.86	O
ATOM	1637	N	LYS	B	652	36.925	-1.165	28.109	1.00	5.25	N
ATOM	1638	CA	LYS	B	652	36.770	-2.429	28.776	1.00	7.08	C
ATOM	1639	CB	LYS	B	652	36.116	-2.190	30.135	1.00	9.45	C
ATOM	1640	CG	LYS	B	652	36.103	-3.327	31.124	1.00	9.85	C
ATOM	1641	CD	LYS	B	652	35.793	-2.711	32.483	1.00	8.46	C
ATOM	1642	CE	LYS	B	652	34.602	-3.426	33.172	1.00	11.02	C
ATOM	1643	NZ	LYS	B	652	34.713	-4.916	33.235	1.00	10.84	N
ATOM	1644	C	LYS	B	652	35.971	-3.380	27.910	1.00	6.24	C
ATOM	1645	O	LYS	B	652	36.417	-4.472	27.586	1.00	6.42	O
ATOM	1646	N	LYS	B	653	34.803	-2.965	27.484	1.00	6.01	N
ATOM	1647	CA	LYS	B	653	34.039	-3.842	26.566	1.00	5.79	C
ATOM	1648	CB	LYS	B	653	32.592	-3.355	26.388	1.00	6.75	C
ATOM	1649	CG	LYS	B	653	31.683	-3.588	27.623	1.00	6.98	C
ATOM	1650	CD	LYS	B	653	30.444	-2.803	27.531	1.00	9.41	C
ATOM	1651	CE	LYS	B	653	29.457	-3.240	28.518	1.00	9.56	C
ATOM	1652	NZ	LYS	B	653	29.069	-4.552	28.071	1.00	16.84	N
ATOM	1653	C	LYS	B	653	34.665	-4.068	25.177	1.00	5.15	C
ATOM	1654	O	LYS	B	653	34.680	-5.204	24.665	1.00	5.64	O
ATOM	1655	N	VAL	B	654	35.172	-3.033	24.528	1.00	3.96	N
ATOM	1656	CA	VAL	B	654	35.796	-3.311	23.240	1.00	4.21	C
ATOM	1657	CB	VAL	B	654	36.340	-2.025	22.582	1.00	3.09	C
ATOM	1658	CG1	VAL	B	654	37.138	-2.320	21.425	1.00	4.47	C
ATOM	1659	CG2	VAL	B	654	35.261	-1.175	22.068	1.00	3.53	C
ATOM	1660	C	VAL	B	654	36.923	-4.399	23.425	1.00	5.38	C
ATOM	1661	O	VAL	B	654	37.162	-5.194	22.517	1.00	5.50	O
ATOM	1662	N	TYR	B	655	37.606	-4.433	24.579	1.00	4.72	N
ATOM	1663	CA	TYR	B	655	38.644	-5.454	24.769	1.00	6.51	C
ATOM	1664	CB	TYR	B	655	39.505	-5.204	26.019	1.00	6.11	C
ATOM	1665	CG	TYR	B	655	40.456	-4.016	25.925	1.00	9.57	C
ATOM	1666	CD1	TYR	B	655	41.074	-3.656	24.712	1.00	10.61	C
ATOM	1667	CE1	TYR	B	655	41.943	-2.567	24.654	1.00	12.73	C
ATOM	1668	CZ	TYR	B	655	42.195	-1.858	25.839	1.00	13.88	C
ATOM	1669	OH	TYR	B	655	43.039	-0.758	25.867	1.00	17.21	O

ATOM	1670	CE2	TYR	B	655	41.577	-2.206	27.021	1.00	8.69	C
ATOM	1671	CD2	TYR	B	655	40.725	-3.241	27.055	1.00	9.00	C
ATOM	1672	C	TYR	B	655	38.074	-6.888	24.825	1.00	6.04	C
ATOM	1673	O	TYR	B	655	38.605	-7.806	24.221	1.00	6.92	O
ATOM	1674	N	ARG	B	656	36.985	-7.059	25.528	1.00	5.36	N
ATOM	1675	CA	ARG	B	656	36.402	-8.358	25.720	1.00	6.12	C
ATOM	1676	CB	ARG	B	656	35.157	-8.238	26.641	1.00	5.83	C
ATOM	1677	CG	ARG	B	656	34.955	-9.400	27.555	1.00	9.85	C
ATOM	1678	CD	ARG	B	656	33.527	-9.895	27.730	1.00	14.72	C
ATOM	1679	NE	ARG	B	656	33.278	-10.215	29.135	1.00	19.73	N
ATOM	1680	CZ	ARG	B	656	32.174	-10.816	29.568	1.00	23.51	C
ATOM	1681	NH1	ARG	B	656	31.217	-11.188	28.707	1.00	26.59	N
ATOM	1682	NH2	ARG	B	656	32.021	-11.056	30.851	1.00	19.55	N
ATOM	1683	C	ARG	B	656	36.008	-8.885	24.362	1.00	5.96	C
ATOM	1684	O	ARG	B	656	36.360	-9.999	24.006	1.00	5.87	O
ATOM	1685	N	LEU	B	657	35.272	-8.056	23.612	1.00	6.37	N
ATOM	1686	CA	LEU	B	657	34.794	-8.416	22.293	1.00	6.12	C
ATOM	1687	CB	LEU	B	657	34.122	-7.226	21.632	1.00	5.46	C
ATOM	1688	CG	LEU	B	657	32.951	-7.388	20.640	1.00	7.16	C
ATOM	1689	CD1	LEU	B	657	33.118	-6.470	19.460	1.00	2.00	C
ATOM	1690	CD2	LEU	B	657	32.700	-8.824	20.156	1.00	5.57	C
ATOM	1691	C	LEU	B	657	36.009	-8.820	21.465	1.00	6.67	C
ATOM	1692	O	LEU	B	657	36.065	-9.905	20.924	1.00	6.08	O
ATOM	1693	N	ALA	B	658	37.004	-7.943	21.405	1.00	7.27	N
ATOM	1694	CA	ALA	B	658	38.156	-8.168	20.556	1.00	7.68	C
ATOM	1695	CB	ALA	B	658	39.093	-7.045	20.658	1.00	9.00	C
ATOM	1696	C	ALA	B	658	38.893	-9.422	20.884	1.00	8.43	C
ATOM	1697	O	ALA	B	658	39.271	-10.196	19.981	1.00	8.28	O
ATOM	1698	N	TYR	B	659	39.143	-9.615	22.174	1.00	8.68	N
ATOM	1699	CA	TYR	B	659	39.850	-10.806	22.595	1.00	8.59	C
ATOM	1700	CB	TYR	B	659	40.177	-10.769	24.087	1.00	8.82	C
ATOM	1701	CG	TYR	B	659	40.775	-12.110	24.491	1.00	11.54	C
ATOM	1702	CD1	TYR	B	659	42.087	-12.435	24.133	1.00	7.96	C
ATOM	1703	CE1	TYR	B	659	42.608	-13.629	24.463	1.00	12.41	C
ATOM	1704	CZ	TYR	B	659	41.822	-14.579	25.146	1.00	14.10	C
ATOM	1705	OH	TYR	B	659	42.353	-15.803	25.433	1.00	10.91	O
ATOM	1706	CE2	TYR	B	659	40.511	-14.296	25.495	1.00	12.41	C
ATOM	1707	CD2	TYR	B	659	39.996	-13.070	25.164	1.00	11.29	C

ATOM	1708	C	TYR	B	659	39.053	-12.090	22.229	1.00	8.10	C
ATOM	1709	O	TYR	B	659	39.591	-13.017	21.663	1.00	7.91	O
ATOM	1710	N	LEU	B	660	37.773	-12.143	22.548	1.00	8.11	N
ATOM	1711	CA	LEU	B	660	36.976	-13.330	22.205	1.00	8.99	C
ATOM	1712	CB	LEU	B	660	35.494	-13.149	22.601	1.00	8.89	C
ATOM	1713	CG	LEU	B	660	35.270	-13.204	24.110	1.00	9.33	C
ATOM	1714	CD1	LEU	B	660	33.943	-12.684	24.547	1.00	9.61	C
ATOM	1715	CD2	LEU	B	660	35.439	-14.643	24.553	1.00	9.83	C
ATOM	1716	C	LEU	B	660	37.054	-13.675	20.721	1.00	9.42	C
ATOM	1717	O	LEU	B	660	37.057	-14.831	20.349	1.00	9.34	O
ATOM	1718	N	ARG	B	661	37.054	-12.663	19.860	1.00	9.71	N
ATOM	1719	CA	ARG	B	661	37.050	-12.968	18.462	1.00	10.45	C
ATOM	1720	CB	ARG	B	661	36.608	-11.793	17.653	1.00	8.53	C
ATOM	1721	CG	ARG	B	661	35.229	-11.304	17.915	1.00	7.97	C
ATOM	1722	CD	ARG	B	661	34.886	-10.027	17.178	1.00	3.76	C
ATOM	1723	NE	ARG	B	661	33.472	-9.762	16.983	1.00	2.70	N
ATOM	1724	CZ	ARG	B	661	32.973	-8.629	16.467	1.00	3.60	C
ATOM	1725	NH1	ARG	B	661	33.784	-7.652	16.053	1.00	3.87	N
ATOM	1726	NH2	ARG	B	661	31.652	-8.468	16.330	1.00	2.00	N
ATOM	1727	C	ARG	B	661	38.478	-13.448	18.096	1.00	12.78	C
ATOM	1728	O	ARG	B	661	38.625	-14.338	17.273	1.00	13.90	O
ATOM	1729	N	LEU	B	662	39.508	-12.879	18.735	1.00	13.10	N
ATOM	1730	CA	LEU	B	662	40.902	-13.230	18.462	1.00	13.72	C
ATOM	1731	CB	LEU	B	662	41.803	-12.308	19.265	1.00	13.06	C
ATOM	1732	CG	LEU	B	662	43.286	-12.110	18.918	1.00	14.40	C
ATOM	1733	CD1	LEU	B	662	44.132	-12.325	20.086	1.00	9.20	C
ATOM	1734	CD2	LEU	B	662	43.829	-12.854	17.630	1.00	15.62	C
ATOM	1735	C	LEU	B	662	41.198	-14.658	18.904	1.00	15.28	C
ATOM	1736	O	LEU	B	662	41.900	-15.448	18.206	1.00	15.63	O
ATOM	1737	N	ASN	B	663	40.656	-14.980	20.082	1.00	15.58	N
ATOM	1738	CA	ASN	B	663	40.829	-16.268	20.666	1.00	15.36	C
ATOM	1739	CB	ASN	B	663	40.287	-16.291	22.090	1.00	15.75	C
ATOM	1740	CG	ASN	B	663	40.059	-17.727	22.606	1.00	16.02	C
ATOM	1741	OD1	ASN	B	663	38.985	-18.274	22.388	1.00	16.31	O
ATOM	1742	ND2	ASN	B	663	41.057	-18.320	23.284	1.00	9.15	N
ATOM	1743	C	ASN	B	663	40.143	-17.296	19.840	1.00	15.24	C
ATOM	1744	O	ASN	B	663	40.592	-18.403	19.771	1.00	15.75	O
ATOM	1745	N	THR	B	664	39.030	-16.930	19.225	1.00	15.92	N

ATOM	1746	CA	THR	B	664	38.274	-17.868	18.396	1.00	15.65	C
ATOM	1747	CB	THR	B	664	36.934	-17.267	17.986	1.00	16.03	C
ATOM	1748	OG1	THR	B	664	36.179	-16.882	19.145	1.00	18.60	O
ATOM	1749	CG2	THR	B	664	36.076	-18.315	17.271	1.00	12.83	C
ATOM	1750	C	THR	B	664	39.059	-18.201	17.126	1.00	15.89	C
ATOM	1751	O	THR	B	664	39.095	-19.335	16.740	1.00	15.40	O
ATOM	1752	N	LEU	B	665	39.661	-17.208	16.472	1.00	16.10	N
ATOM	1753	CA	LEU	B	665	40.453	-17.463	15.290	1.00	17.99	C
ATOM	1754	CB	LEU	B	665	40.700	-16.171	14.515	1.00	18.03	C
ATOM	1755	CG	LEU	B	665	39.504	-15.473	13.840	1.00	17.81	C
ATOM	1756	CD1	LEU	B	665	39.932	-14.082	13.322	1.00	14.11	C
ATOM	1757	CD2	LEU	B	665	38.978	-16.273	12.715	1.00	15.62	C
ATOM	1758	C	LEU	B	665	41.816	-18.142	15.599	1.00	18.90	C
ATOM	1759	O	LEU	B	665	42.290	-18.978	14.843	1.00	18.38	O
ATOM	1760	N	CYS	B	666	42.452	-17.769	16.702	1.00	19.38	N
ATOM	1761	CA	CYS	B	666	43.727	-18.381	17.036	1.00	19.52	C
ATOM	1762	CB	CYS	B	666	44.435	-17.649	18.192	1.00	20.43	C
ATOM	1763	SG	CYS	B	666	45.104	-16.057	17.678	1.00	19.13	S
ATOM	1764	C	CYS	B	666	43.614	-19.808	17.430	1.00	19.42	C
ATOM	1765	O	CYS	B	666	44.601	-20.549	17.260	1.00	19.57	O
ATOM	1766	N	GLU	B	667	42.463	-20.191	18.009	1.00	18.97	N
ATOM	1767	CA	GLU	B	667	42.273	-21.576	18.478	1.00	18.84	C
ATOM	1768	CB	GLU	B	667	41.170	-21.680	19.536	1.00	18.36	C
ATOM	1769	CG	GLU	B	667	40.892	-23.085	20.048	1.00	17.77	C
ATOM	1770	CD	GLU	B	667	40.404	-23.151	21.526	1.00	18.28	C
ATOM	1771	OE1	GLU	B	667	39.851	-24.235	21.937	1.00	12.51	O
ATOM	1772	OE2	GLU	B	667	40.586	-22.126	22.277	1.00	16.34	O
ATOM	1773	C	GLU	B	667	42.019	-22.508	17.291	1.00	19.46	C
ATOM	1774	O	GLU	B	667	42.257	-23.691	17.387	1.00	20.81	O
ATOM	1775	N	ARG	B	668	41.558	-21.979	16.166	1.00	18.39	N
ATOM	1776	CA	ARG	B	668	41.330	-22.817	15.012	1.00	18.41	C
ATOM	1777	CB	ARG	B	668	40.005	-22.454	14.376	1.00	19.07	C
ATOM	1778	CG	ARG	B	668	38.775	-22.369	15.341	1.00	20.80	C
ATOM	1779	CD	ARG	B	668	37.477	-21.891	14.616	1.00	19.53	C
ATOM	1780	NE	ARG	B	668	36.292	-21.858	15.484	1.00	23.37	N
ATOM	1781	CZ	ARG	B	668	35.058	-21.419	15.127	1.00	22.67	C
ATOM	1782	NH1	ARG	B	668	34.778	-20.972	13.896	1.00	20.39	N
ATOM	1783	NH2	ARG	B	668	34.094	-21.407	16.035	1.00	20.67	N

ATOM	1784	C	ARG	B	668	42.450	-22.719	13.950	1.00	18.34	C
ATOM	1785	O	ARG	B	668	42.651	-23.613	13.122	1.00	17.26	O
ATOM	1786	N	LEU	B	669	43.206	-21.630	13.988	1.00	18.42	N
ATOM	1787	CA	LEU	B	669	44.255	-21.413	13.001	1.00	18.63	C
ATOM	1788	CB	LEU	B	669	44.105	-19.999	12.412	1.00	19.29	C
ATOM	1789	CG	LEU	B	669	43.433	-19.874	11.029	1.00	20.70	C
ATOM	1790	CD1	LEU	B	669	42.191	-20.771	10.861	1.00	18.65	C
ATOM	1791	CD2	LEU	B	669	43.167	-18.385	10.606	1.00	15.39	C
ATOM	1792	C	LEU	B	669	45.677	-21.649	13.553	1.00	18.31	C
ATOM	1793	O	LEU	B	669	46.559	-22.131	12.850	1.00	17.46	O
ATOM	1794	N	LEU	B	670	45.892	-21.320	14.819	1.00	17.97	N
ATOM	1795	CA	LEU	B	670	47.206	-21.450	15.382	1.00	18.50	C
ATOM	1796	CB	LEU	B	670	47.699	-20.070	15.762	1.00	18.75	C
ATOM	1797	CG	LEU	B	670	47.828	-19.118	14.568	1.00	17.36	C
ATOM	1798	CD1	LEU	B	670	48.413	-17.828	15.007	1.00	15.48	C
ATOM	1799	CD2	LEU	B	670	48.698	-19.778	13.477	1.00	14.62	C
ATOM	1800	C	LEU	B	670	47.340	-22.401	16.552	1.00	19.33	C
ATOM	1801	O	LEU	B	670	48.121	-22.162	17.448	1.00	19.41	O
ATOM	1802	N	SER	B	671	46.646	-23.529	16.514	1.00	21.39	N
ATOM	1803	CA	SER	B	671	46.704	-24.470	17.632	1.00	23.09	C
ATOM	1804	CB	SER	B	671	45.665	-25.575	17.484	1.00	22.45	C
ATOM	1805	OG	SER	B	671	45.803	-26.222	16.227	1.00	23.79	O
ATOM	1806	C	SER	B	671	48.081	-25.084	17.765	1.00	24.29	C
ATOM	1807	O	SER	B	671	48.467	-25.474	18.858	1.00	24.66	O
ATOM	1808	N	GLU	B	672	48.806	-25.180	16.644	1.00	25.50	N
ATOM	1809	CA	GLU	B	672	50.152	-25.749	16.637	1.00	25.94	C
ATOM	1810	CB	GLU	B	672	50.715	-25.898	15.221	1.00	27.18	C
ATOM	1811	CG	GLU	B	672	49.983	-26.842	14.267	1.00	31.37	C
ATOM	1812	CD	GLU	B	672	50.420	-26.667	12.787	1.00	36.21	C
ATOM	1813	OE1	GLU	B	672	50.113	-25.634	12.135	1.00	34.47	O
ATOM	1814	OE2	GLU	B	672	51.058	-27.605	12.247	1.00	40.18	O
ATOM	1815	C	GLU	B	672	51.097	-24.868	17.431	1.00	25.14	C
ATOM	1816	O	GLU	B	672	52.048	-25.379	18.006	1.00	25.38	O
ATOM	1817	N	HIS	B	673	50.867	-23.548	17.439	1.00	24.39	N
ATOM	1818	CA	HIS	B	673	51.727	-22.613	18.226	1.00	23.25	C
ATOM	1819	CB	HIS	B	673	52.507	-21.670	17.308	1.00	22.74	C
ATOM	1820	CG	HIS	B	673	52.982	-22.304	16.035	1.00	24.74	C
ATOM	1821	ND1	HIS	B	673	52.234	-22.309	14.874	1.00	23.69	N

ATOM	1822	CE1	HIS	B	673	52.909	-22.931	13.920	1.00	23.68	C
ATOM	1823	NE2	HIS	B	673	54.075	-23.316	14.413	1.00	23.92	N
ATOM	1824	CD2	HIS	B	673	54.142	-22.947	15.737	1.00	25.13	C
ATOM	1825	C	HIS	B	673	50.904	-21.811	19.255	1.00	21.86	C
ATOM	1826	O	HIS	B	673	50.723	-20.598	19.131	1.00	21.72	O
ATOM	1827	N	PRO	B	674	50.422	-22.506	20.274	1.00	20.75	N
ATOM	1828	CA	PRO	B	674	49.579	-21.913	21.309	1.00	19.67	C
ATOM	1829	CB	PRO	B	674	49.540	-23.021	22.379	1.00	19.92	C
ATOM	1830	CG	PRO	B	674	49.687	-24.247	21.623	1.00	19.13	C
ATOM	1831	CD	PRO	B	674	50.691	-23.934	20.547	1.00	20.60	C
ATOM	1832	C	PRO	B	674	50.126	-20.630	21.901	1.00	18.69	C
ATOM	1833	O	PRO	B	674	49.369	-19.848	22.443	1.00	18.47	O
ATOM	1834	N	GLU	B	675	51.420	-20.396	21.773	1.00	18.13	N
ATOM	1835	CA	GLU	B	675	51.998	-19.194	22.326	1.00	18.19	C
ATOM	1836	CB	GLU	B	675	53.517	-19.319	22.414	1.00	18.97	C
ATOM	1837	CG	GLU	B	675	54.274	-19.156	21.088	1.00	19.76	C
ATOM	1838	CD	GLU	B	675	54.239	-20.376	20.186	1.00	18.67	C
ATOM	1839	OE1	GLU	B	675	53.642	-21.410	20.560	1.00	16.34	O
ATOM	1840	OE2	GLU	B	675	54.824	-20.283	19.085	1.00	18.78	O
ATOM	1841	C	GLU	B	675	51.657	-17.940	21.548	1.00	17.58	C
ATOM	1842	O	GLU	B	675	51.660	-16.886	22.121	1.00	18.20	O
ATOM	1843	N	LEU	B	676	51.382	-18.030	20.250	1.00	16.44	N
ATOM	1844	CA	LEU	B	676	51.143	-16.803	19.469	1.00	15.70	C
ATOM	1845	CB	LEU	B	676	51.006	-17.104	17.965	1.00	15.18	C
ATOM	1846	CG	LEU	B	676	52.243	-17.715	17.348	1.00	13.23	C
ATOM	1847	CD1	LEU	B	676	52.008	-17.973	15.866	1.00	12.22	C
ATOM	1848	CD2	LEU	B	676	53.405	-16.751	17.566	1.00	8.01	C
ATOM	1849	C	LEU	B	676	49.986	-15.898	19.905	1.00	14.78	C
ATOM	1850	O	LEU	B	676	50.038	-14.706	19.703	1.00	14.81	O
ATOM	1851	N	GLU	B	677	48.933	-16.455	20.473	1.00	14.63	N
ATOM	1852	CA	GLU	B	677	47.758	-15.636	20.830	1.00	14.03	C
ATOM	1853	CB	GLU	B	677	46.618	-16.503	21.396	1.00	12.86	C
ATOM	1854	CG	GLU	B	677	45.378	-15.737	21.847	1.00	14.72	C
ATOM	1855	CD	GLU	B	677	44.387	-16.590	22.666	1.00	17.27	C
ATOM	1856	OE1	GLU	B	677	43.557	-17.338	22.098	1.00	15.74	O
ATOM	1857	OE2	GLU	B	677	44.427	-16.530	23.901	1.00	16.88	O
ATOM	1858	C	GLU	B	677	48.062	-14.467	21.749	1.00	13.75	C
ATOM	1859	O	GLU	B	677	47.589	-13.318	21.520	1.00	14.06	O

ATOM	1860	N	HIS	B	678	48.841	-14.733	22.788	1.00	13.20	N
ATOM	1861	CA	HIS	B	678	49.142	-13.689	23.765	1.00	14.08	C
ATOM	1862	CB	HIS	B	678	49.775	-14.274	25.031	1.00	14.28	C
ATOM	1863	CG	HIS	B	678	49.611	-13.422	26.257	1.00	16.75	C
ATOM	1864	ND1	HIS	B	678	48.616	-12.466	26.386	1.00	18.50	N
ATOM	1865	CE1	HIS	B	678	48.698	-11.904	27.580	1.00	17.30	C
ATOM	1866	NE2	HIS	B	678	49.721	-12.439	28.220	1.00	16.02	N
ATOM	1867	CD2	HIS	B	678	50.306	-13.393	27.418	1.00	15.51	C
ATOM	1868	C	HIS	B	678	50.019	-12.585	23.184	1.00	13.46	C
ATOM	1869	O	HIS	B	678	49.895	-11.445	23.578	1.00	13.27	O
ATOM	1870	N	ILE	B	679	50.907	-12.922	22.248	1.00	13.66	N
ATOM	1871	CA	ILE	B	679	51.758	-11.903	21.623	1.00	13.87	C
ATOM	1872	CB	ILE	B	679	52.940	-12.548	20.884	1.00	14.37	C
ATOM	1873	CG1	ILE	B	679	53.840	-13.349	21.826	1.00	15.38	C
ATOM	1874	CD1	ILE	B	679	54.959	-14.175	21.105	1.00	11.31	C
ATOM	1875	CG2	ILE	B	679	53.795	-11.481	20.210	1.00	16.19	C
ATOM	1876	C	ILE	B	679	50.914	-11.020	20.660	1.00	13.66	C
ATOM	1877	O	ILE	B	679	51.018	-9.776	20.652	1.00	12.95	O
ATOM	1878	N	ILE	B	680	50.072	-11.675	19.860	1.00	12.55	N
ATOM	1879	CA	ILE	B	680	49.162	-10.987	18.958	1.00	11.61	C
ATOM	1880	CB	ILE	B	680	48.355	-12.008	18.110	1.00	11.65	C
ATOM	1881	CG1	ILE	B	680	49.280	-12.924	17.344	1.00	9.78	C
ATOM	1882	CD1	ILE	B	680	48.562	-13.950	16.468	1.00	9.87	C
ATOM	1883	CG2	ILE	B	680	47.473	-11.289	17.076	1.00	12.42	C
ATOM	1884	C	ILE	B	680	48.199	-10.085	19.727	1.00	11.07	C
ATOM	1885	O	ILE	B	680	47.921	-8.939	19.315	1.00	10.14	O
ATOM	1886	N	TRP	B	681	47.693	-10.596	20.844	1.00	10.25	N
ATOM	1887	CA	TRP	B	681	46.736	-9.810	21.625	1.00	9.98	C
ATOM	1888	CB	TRP	B	681	46.107	-10.594	22.784	1.00	10.30	C
ATOM	1889	CG	TRP	B	681	45.516	-9.703	23.783	1.00	10.20	C
ATOM	1890	CD1	TRP	B	681	45.943	-9.489	25.083	1.00	8.14	C
ATOM	1891	NE1	TRP	B	681	45.123	-8.570	25.691	1.00	11.57	N
ATOM	1892	CE2	TRP	B	681	44.174	-8.153	24.780	1.00	10.57	C
ATOM	1893	CD2	TRP	B	681	44.396	-8.851	23.580	1.00	12.27	C
ATOM	1894	CE3	TRP	B	681	43.548	-8.595	22.486	1.00	12.34	C
ATOM	1895	CZ3	TRP	B	681	42.549	-7.671	22.623	1.00	8.26	C
ATOM	1896	CH2	TRP	B	681	42.385	-6.984	23.815	1.00	9.93	C
ATOM	1897	CZ2	TRP	B	681	43.188	-7.210	24.900	1.00	8.58	C

ATOM	1898	C	TRP	B	681	47.427	-8.596	22.136	1.00	9.60	C
ATOM	1899	O	TRP	B	681	46.818	-7.521	22.282	1.00	10.07	O
ATOM	1900	N	THR	B	682	48.710	-8.757	22.431	1.00	9.03	N
ATOM	1901	CA	THR	B	682	49.523	-7.629	22.897	1.00	7.57	C
ATOM	1902	CB	THR	B	682	50.887	-8.117	23.316	1.00	7.89	C
ATOM	1903	OG1	THR	B	682	50.760	-8.912	24.499	1.00	7.20	O
ATOM	1904	CG2	THR	B	682	51.776	-6.939	23.723	1.00	9.26	C
ATOM	1905	C	THR	B	682	49.664	-6.547	21.858	1.00	5.80	C
ATOM	1906	O	THR	B	682	49.522	-5.428	22.192	1.00	5.05	O
ATOM	1907	N	LEU	B	683	50.010	-6.900	20.621	1.00	5.57	N
ATOM	1908	CA	LEU	B	683	50.082	-5.949	19.482	1.00	5.60	C
ATOM	1909	CB	LEU	B	683	50.485	-6.672	18.233	1.00	4.78	C
ATOM	1910	CG	LEU	B	683	51.117	-5.923	17.106	1.00	6.57	C
ATOM	1911	CD1	LEU	B	683	50.996	-6.590	15.661	1.00	4.62	C
ATOM	1912	CD2	LEU	B	683	50.646	-4.513	17.107	1.00	8.25	C
ATOM	1913	C	LEU	B	683	48.706	-5.331	19.208	1.00	5.57	C
ATOM	1914	O	LEU	B	683	48.604	-4.143	18.911	1.00	4.88	O
ATOM	1915	N	PHE	B	684	47.659	-6.158	19.336	1.00	6.06	N
ATOM	1916	CA	PHE	B	684	46.291	-5.766	19.089	1.00	6.35	C
ATOM	1917	CB	PHE	B	684	45.365	-6.971	19.277	1.00	6.20	C
ATOM	1918	CG	PHE	B	684	43.963	-6.775	18.749	1.00	5.04	C
ATOM	1919	CD1	PHE	B	684	43.516	-5.561	18.371	1.00	5.84	C
ATOM	1920	CE1	PHE	B	684	42.232	-5.363	17.912	1.00	9.04	C
ATOM	1921	CZ	PHE	B	684	41.368	-6.426	17.831	1.00	10.79	C
ATOM	1922	CE2	PHE	B	684	41.793	-7.674	18.174	1.00	10.95	C
ATOM	1923	CD2	PHE	B	684	43.096	-7.845	18.653	1.00	10.41	C
ATOM	1924	C	PHE	B	684	45.885	-4.661	20.010	1.00	6.76	C
ATOM	1925	O	PHE	B	684	45.351	-3.634	19.545	1.00	7.52	O
ATOM	1926	N	GLN	B	685	46.183	-4.856	21.293	1.00	6.72	N
ATOM	1927	CA	GLN	B	685	45.785	-3.957	22.379	1.00	6.81	C
ATOM	1928	CB	GLN	B	685	45.903	-4.668	23.756	1.00	7.65	C
ATOM	1929	CG	GLN	B	685	45.463	-3.884	25.038	1.00	10.43	C
ATOM	1930	CD	GLN	B	685	46.325	-2.667	25.299	1.00	16.01	C
ATOM	1931	OE1	GLN	B	685	45.818	-1.596	25.619	1.00	13.41	O
ATOM	1932	NE2	GLN	B	685	47.650	-2.813	25.090	1.00	17.77	N
ATOM	1933	C	GLN	B	685	46.597	-2.708	22.317	1.00	6.15	C
ATOM	1934	O	GLN	B	685	46.095	-1.608	22.604	1.00	5.65	O
ATOM	1935	N	HIS	B	686	47.843	-2.870	21.897	1.00	5.79	N

ATOM	1936	CA	HIS	B	686	48.776	-1.748	21.793	1.00	6.80	C
ATOM	1937	CB	HIS	B	686	50.212	-2.230	21.429	1.00	6.29	C
ATOM	1938	CG	HIS	B	686	51.124	-1.132	20.934	1.00	12.07	C
ATOM	1939	ND1	HIS	B	686	51.758	-0.238	21.781	1.00	17.34	N
ATOM	1940	CE1	HIS	B	686	52.481	0.616	21.068	1.00	14.84	C
ATOM	1941	NE2	HIS	B	686	52.355	0.303	19.791	1.00	13.76	N
ATOM	1942	CD2	HIS	B	686	51.509	-0.783	19.676	1.00	13.72	C
ATOM	1943	C	HIS	B	686	48.241	-0.747	20.772	1.00	6.86	C
ATOM	1944	O	HIS	B	686	48.443	0.473	20.897	1.00	5.59	O
ATOM	1945	N	THR	B	687	47.531	-1.302	19.791	1.00	6.24	N
ATOM	1946	CA	THR	B	687	47.058	-0.557	18.692	1.00	7.58	C
ATOM	1947	CB	THR	B	687	46.784	-1.518	17.502	1.00	8.36	C
ATOM	1948	OG1	THR	B	687	48.012	-2.196	17.143	1.00	6.50	O
ATOM	1949	CG2	THR	B	687	46.448	-0.754	16.252	1.00	6.00	C
ATOM	1950	C	THR	B	687	45.871	0.216	19.119	1.00	8.56	C
ATOM	1951	O	THR	B	687	45.839	1.429	19.017	1.00	10.02	O
ATOM	1952	N	LEU	B	688	44.898	-0.482	19.673	1.00	9.41	N
ATOM	1953	CA	LEU	B	688	43.666	0.139	20.069	1.00	8.15	C
ATOM	1954	CB	LEU	B	688	42.762	-0.907	20.687	1.00	7.39	C
ATOM	1955	CG	LEU	B	688	42.153	-1.890	19.723	1.00	10.18	C
ATOM	1956	CD1	LEU	B	688	41.445	-3.058	20.415	1.00	7.27	C
ATOM	1957	CD2	LEU	B	688	41.142	-1.098	18.791	1.00	13.68	C
ATOM	1958	C	LEU	B	688	43.962	1.272	21.036	1.00	8.20	C
ATOM	1959	O	LEU	B	688	43.227	2.296	21.085	1.00	7.09	O
ATOM	1960	N	GLN	B	689	45.030	1.084	21.812	1.00	8.37	N
ATOM	1961	CA	GLN	B	689	45.360	2.012	22.883	1.00	9.31	C
ATOM	1962	CB	GLN	B	689	45.965	1.285	24.062	1.00	9.91	C
ATOM	1963	CG	GLN	B	689	46.488	2.136	25.193	1.00	11.42	C
ATOM	1964	CD	GLN	B	689	47.388	1.309	26.139	1.00	17.91	C
ATOM	1965	OE1	GLN	B	689	47.428	1.509	27.368	1.00	16.41	O
ATOM	1966	NE2	GLN	B	689	48.116	0.373	25.548	1.00	22.03	N
ATOM	1967	C	GLN	B	689	46.291	3.107	22.475	1.00	10.03	C
ATOM	1968	O	GLN	B	689	46.151	4.202	22.972	1.00	10.38	O
ATOM	1969	N	ASN	B	690	47.242	2.842	21.585	1.00	10.31	N
ATOM	1970	CA	ASN	B	690	48.195	3.873	21.243	1.00	10.87	C
ATOM	1971	CB	ASN	B	690	49.594	3.477	21.680	1.00	11.41	C
ATOM	1972	CG	ASN	B	690	49.655	3.038	23.163	1.00	14.58	C
ATOM	1973	OD1	ASN	B	690	49.287	3.797	24.079	1.00	12.40	O

ATOM	1974	ND2	ASN	B	690	50.129	1.806	23.395	1.00	13.56	N
ATOM	1975	C	ASN	B	690	48.200	4.283	19.791	1.00	11.32	C
ATOM	1976	O	ASN	B	690	48.675	5.346	19.472	1.00	12.34	O
ATOM	1977	N	GLU	B	691	47.670	3.471	18.897	1.00	11.49	N
ATOM	1978	CA	GLU	B	691	47.629	3.873	17.493	1.00	12.32	C
ATOM	1979	CB	GLU	B	691	48.418	2.895	16.589	1.00	13.24	C
ATOM	1980	CG	GLU	B	691	49.824	2.554	17.042	1.00	16.51	C
ATOM	1981	CD	GLU	B	691	50.774	3.763	16.964	1.00	27.49	C
ATOM	1982	OE1	GLU	B	691	50.583	4.649	16.071	1.00	28.02	O
ATOM	1983	OE2	GLU	B	691	51.722	3.845	17.795	1.00	27.57	O
ATOM	1984	C	GLU	B	691	46.173	3.941	17.054	1.00	11.32	C
ATOM	1985	O	GLU	B	691	45.826	3.491	15.982	1.00	9.71	O
ATOM	1986	N	TYR	B	692	45.346	4.520	17.925	1.00	12.17	N
ATOM	1987	CA	TYR	B	692	43.892	4.662	17.749	1.00	11.54	C
ATOM	1988	CB	TYR	B	692	43.246	5.296	18.968	1.00	10.36	C
ATOM	1989	CG	TYR	B	692	43.781	6.634	19.276	1.00	12.35	C
ATOM	1990	CD1	TYR	B	692	43.456	7.724	18.465	1.00	13.10	C
ATOM	1991	CE1	TYR	B	692	43.952	8.952	18.712	1.00	12.96	C
ATOM	1992	CZ	TYR	B	692	44.790	9.139	19.800	1.00	15.72	C
ATOM	1993	OH	TYR	B	692	45.273	10.416	20.038	1.00	18.87	O
ATOM	1994	CE2	TYR	B	692	45.130	8.076	20.641	1.00	12.33	C
ATOM	1995	CD2	TYR	B	692	44.643	6.833	20.368	1.00	10.45	C
ATOM	1996	C	TYR	B	692	43.456	5.375	16.481	1.00	11.74	C
ATOM	1997	O	TYR	B	692	42.342	5.147	16.015	1.00	12.21	O
ATOM	1998	N	GLU	B	693	44.334	6.181	15.881	1.00	11.26	N
ATOM	1999	CA	GLU	B	693	43.993	6.843	14.644	1.00	10.21	C
ATOM	2000	CB	GLU	B	693	45.024	7.880	14.262	1.00	10.93	C
ATOM	2001	CG	GLU	B	693	44.958	9.126	15.116	1.00	12.97	C
ATOM	2002	CD	GLU	B	693	43.629	9.809	15.027	1.00	16.35	C
ATOM	2003	OE1	GLU	B	693	43.221	10.421	16.037	1.00	22.86	O
ATOM	2004	OE2	GLU	B	693	42.974	9.751	13.961	1.00	15.98	O
ATOM	2005	C	GLU	B	693	43.839	5.846	13.532	1.00	9.33	C
ATOM	2006	O	GLU	B	693	43.184	6.125	12.529	1.00	10.07	O
ATOM	2007	N	LEU	B	694	44.370	4.664	13.729	1.00	7.38	N
ATOM	2008	CA	LEU	B	694	44.294	3.595	12.747	1.00	7.01	C
ATOM	2009	CB	LEU	B	694	45.194	2.459	13.250	1.00	8.21	C
ATOM	2010	CG	LEU	B	694	46.133	1.851	12.255	1.00	11.49	C
ATOM	2011	CD1	LEU	B	694	46.625	2.906	11.273	1.00	11.62	C

ATOM	2012	CD2	LEU	B	694	47.261	1.293	13.091	1.00	12.03	C
ATOM	2013	C	LEU	B	694	42.880	3.049	12.604	1.00	6.18	C
ATOM	2014	O	LEU	B	694	42.537	2.492	11.620	1.00	4.81	O
ATOM	2015	N	MET	B	695	42.079	3.163	13.645	1.00	6.55	N
ATOM	2016	CA	MET	B	695	40.705	2.688	13.639	1.00	6.27	C
ATOM	2017	CB	MET	B	695	40.166	2.596	15.082	1.00	7.54	C
ATOM	2018	CG	MET	B	695	40.634	1.332	15.836	1.00	9.37	C
ATOM	2019	SD	MET	B	695	39.938	-0.166	15.166	1.00	7.22	S
ATOM	2020	CE	MET	B	695	38.323	0.077	15.495	1.00	2.00	C
ATOM	2021	C	MET	B	695	39.780	3.627	12.933	1.00	5.88	C
ATOM	2022	O	MET	B	695	38.662	3.212	12.616	1.00	5.11	O
ATOM	2023	N	ARG	B	696	40.219	4.874	12.705	1.00	5.14	N
ATOM	2024	CA	ARG	B	696	39.358	5.925	12.159	1.00	5.59	C
ATOM	2025	CB	ARG	B	696	40.136	7.200	11.947	1.00	6.29	C
ATOM	2026	CG	ARG	B	696	39.302	8.469	11.978	1.00	6.47	C
ATOM	2027	CD	ARG	B	696	40.166	9.744	11.848	1.00	8.31	C
ATOM	2028	NE	ARG	B	696	39.304	10.900	12.043	1.00	13.20	N
ATOM	2029	CZ	ARG	B	696	39.133	11.587	13.185	1.00	9.34	C
ATOM	2030	NH1	ARG	B	696	39.826	11.314	14.278	1.00	3.82	N
ATOM	2031	NH2	ARG	B	696	38.279	12.606	13.177	1.00	9.75	N
ATOM	2032	C	ARG	B	696	38.683	5.569	10.866	1.00	5.88	C
ATOM	2033	O	ARG	B	696	39.321	5.442	9.835	1.00	6.24	O
ATOM	2034	N	ASP	B	697	37.374	5.417	10.909	1.00	5.84	N
ATOM	2035	CA	ASP	B	697	36.620	5.019	9.689	1.00	6.16	C
ATOM	2036	CB	ASP	B	697	36.851	6.024	8.563	1.00	5.37	C
ATOM	2037	CG	ASP	B	697	36.238	7.416	8.830	1.00	5.53	C
ATOM	2038	OD1	ASP	B	697	35.077	7.547	9.309	1.00	7.21	O
ATOM	2039	OD2	ASP	B	697	36.823	8.461	8.482	1.00	3.96	O
ATOM	2040	C	ASP	B	697	36.989	3.586	9.232	1.00	4.52	C
ATOM	2041	O	ASP	B	697	36.893	3.257	8.060	1.00	2.10	O
ATOM	2042	N	ARG	B	698	37.458	2.779	10.173	1.00	2.27	N
ATOM	2043	CA	ARG	B	698	37.862	1.431	9.890	1.00	3.61	C
ATOM	2044	CB	ARG	B	698	39.393	1.335	9.864	1.00	2.00	C
ATOM	2045	CG	ARG	B	698	39.962	1.672	8.510	1.00	7.08	C
ATOM	2046	CD	ARG	B	698	41.414	1.300	8.239	1.00	10.31	C
ATOM	2047	NE	ARG	B	698	42.223	2.334	8.809	1.00	14.26	N
ATOM	2048	CZ	ARG	B	698	42.863	3.260	8.137	1.00	9.60	C
ATOM	2049	NH1	ARG	B	698	42.877	3.272	6.818	1.00	8.71	N

ATOM	2050	NH2	ARG	B	698	43.498	4.171	8.817	1.00	5.51	N
ATOM	2051	C	ARG	B	698	37.198	0.423	10.881	1.00	4.51	C
ATOM	2052	O	ARG	B	698	36.474	0.785	11.830	1.00	5.73	O
ATOM	2053	N	HIS	B	699	37.445	-0.843	10.687	1.00	4.24	N
ATOM	2054	CA	HIS	B	699	36.758	-1.862	11.467	1.00	4.34	C
ATOM	2055	CB	HIS	B	699	36.070	-2.833	10.451	1.00	4.52	C
ATOM	2056	CG	HIS	B	699	35.058	-3.760	11.034	1.00	2.22	C
ATOM	2057	ND1	HIS	B	699	35.386	-4.729	11.964	1.00	3.86	N
ATOM	2058	CE1	HIS	B	699	34.311	-5.460	12.229	1.00	2.00	C
ATOM	2059	NE2	HIS	B	699	33.306	-5.005	11.507	1.00	2.00	N
ATOM	2060	CD2	HIS	B	699	33.746	-3.935	10.758	1.00	2.00	C
ATOM	2061	C	HIS	B	699	37.706	-2.621	12.402	1.00	3.78	C
ATOM	2062	O	HIS	B	699	38.796	-2.946	12.041	1.00	2.51	O
ATOM	2063	N	LEU	B	700	37.226	-2.906	13.608	1.00	3.99	N
ATOM	2064	CA	LEU	B	700	37.962	-3.652	14.592	1.00	4.35	C
ATOM	2065	CB	LEU	B	700	37.015	-4.031	15.713	1.00	3.43	C
ATOM	2066	CG	LEU	B	700	37.467	-4.058	17.177	1.00	2.71	C
ATOM	2067	CD1	LEU	B	700	36.714	-5.193	17.919	1.00	2.00	C
ATOM	2068	CD2	LEU	B	700	38.954	-4.198	17.322	1.00	2.00	C
ATOM	2069	C	LEU	B	700	38.512	-4.994	14.019	1.00	4.85	C
ATOM	2070	O	LEU	B	700	39.607	-5.385	14.340	1.00	3.57	O
ATOM	2071	N	ASP	B	701	37.737	-5.695	13.188	1.00	4.86	N
ATOM	2072	CA	ASP	B	701	38.202	-6.958	12.691	1.00	5.27	C
ATOM	2073	CB	ASP	B	701	37.055	-7.724	12.051	1.00	6.51	C
ATOM	2074	CG	ASP	B	701	35.965	-8.161	13.051	1.00	8.63	C
ATOM	2075	OD1	ASP	B	701	36.140	-8.095	14.300	1.00	8.97	O
ATOM	2076	OD2	ASP	B	701	34.860	-8.568	12.634	1.00	12.11	O
ATOM	2077	C	ASP	B	701	39.392	-6.779	11.683	1.00	5.92	C
ATOM	2078	O	ASP	B	701	40.241	-7.654	11.524	1.00	4.87	O
ATOM	2079	N	GLN	B	702	39.449	-5.650	10.990	1.00	6.01	N
ATOM	2080	CA	GLN	B	702	40.548	-5.398	10.068	1.00	6.04	C
ATOM	2081	CB	GLN	B	702	40.262	-4.162	9.205	1.00	5.99	C
ATOM	2082	CG	GLN	B	702	38.897	-4.192	8.644	1.00	5.27	C
ATOM	2083	CD	GLN	B	702	38.418	-2.903	8.079	1.00	4.96	C
ATOM	2084	OE1	GLN	B	702	38.869	-1.797	8.471	1.00	4.27	O
ATOM	2085	NE2	GLN	B	702	37.475	-3.020	7.135	1.00	3.80	N
ATOM	2086	C	GLN	B	702	41.896	-5.243	10.829	1.00	6.46	C
ATOM	2087	O	GLN	B	702	42.908	-5.756	10.357	1.00	6.12	O

ATOM	2088	N	ILE	B	703	41.899	-4.594	12.002	1.00	5.52	N
ATOM	2089	CA	ILE	B	703	43.105	-4.450	12.777	1.00	6.51	C
ATOM	2090	CB	ILE	B	703	42.911	-3.462	13.974	1.00	8.27	C
ATOM	2091	CG1	ILE	B	703	43.146	-2.006	13.577	1.00	7.52	C
ATOM	2092	CD1	ILE	B	703	42.183	-1.541	12.512	1.00	10.76	C
ATOM	2093	CG2	ILE	B	703	43.838	-3.807	15.102	1.00	5.38	C
ATOM	2094	C	ILE	B	703	43.451	-5.788	13.382	1.00	8.35	C
ATOM	2095	O	ILE	B	703	44.630	-6.094	13.568	1.00	9.15	O
ATOM	2096	N	MET	B	704	42.427	-6.586	13.720	1.00	8.61	N
ATOM	2097	CA	MET	B	704	42.616	-7.906	14.325	1.00	7.76	C
ATOM	2098	CB	MET	B	704	41.284	-8.558	14.722	1.00	7.41	C
ATOM	2099	CG	MET	B	704	41.418	-9.941	15.451	1.00	9.47	C
ATOM	2100	SD	MET	B	704	39.832	-10.902	15.795	1.00	8.72	S
ATOM	2101	CE	MET	B	704	39.200	-10.805	14.093	1.00	2.92	C
ATOM	2102	C	MET	B	704	43.363	-8.835	13.393	1.00	7.58	C
ATOM	2103	O	MET	B	704	44.404	-9.378	13.736	1.00	8.07	O
ATOM	2104	N	MET	B	705	42.825	-9.041	12.207	1.00	7.84	N
ATOM	2105	CA	MET	B	705	43.404	-9.988	11.262	1.00	7.60	C
ATOM	2106	CB	MET	B	705	42.471	-10.153	10.059	1.00	8.87	C
ATOM	2107	CG	MET	B	705	41.137	-10.805	10.290	1.00	7.32	C
ATOM	2108	SD	MET	B	705	40.198	-10.798	8.683	1.00	14.24	S
ATOM	2109	CE	MET	B	705	39.124	-9.281	8.938	1.00	11.08	C
ATOM	2110	C	MET	B	705	44.763	-9.464	10.826	1.00	8.08	C
ATOM	2111	O	MET	B	705	45.637	-10.222	10.558	1.00	7.47	O
ATOM	2112	N	CYS	B	706	44.936	-8.142	10.802	1.00	9.02	N
ATOM	2113	CA	CYS	B	706	46.226	-7.550	10.487	1.00	9.66	C
ATOM	2114	CB	CYS	B	706	46.091	-6.052	10.175	1.00	8.53	C
ATOM	2115	SG	CYS	B	706	45.622	-5.697	8.466	1.00	10.44	S
ATOM	2116	C	CYS	B	706	47.299	-7.794	11.592	1.00	10.66	C
ATOM	2117	O	CYS	B	706	48.520	-7.837	11.297	1.00	10.39	O
ATOM	2118	N	SER	B	707	46.870	-7.931	12.848	1.00	9.97	N
ATOM	2119	CA	SER	B	707	47.837	-8.169	13.873	1.00	10.40	C
ATOM	2120	CB	SER	B	707	47.296	-7.823	15.246	1.00	10.36	C
ATOM	2121	OG	SER	B	707	47.061	-6.435	15.460	1.00	8.24	O
ATOM	2122	C	SER	B	707	48.273	-9.654	13.807	1.00	12.62	C
ATOM	2123	O	SER	B	707	49.474	-9.959	13.991	1.00	11.29	O
ATOM	2124	N	MET	B	708	47.321	-10.563	13.507	1.00	14.70	N
ATOM	2125	CA	MET	B	708	47.649	-12.000	13.401	1.00	16.47	C

ATOM	2126	CB	MET	B	708	46.449	-12.858	13.083	1.00	16.13	C
ATOM	2127	CG	MET	B	708	45.246	-12.592	13.968	1.00	17.64	C
ATOM	2128	SD	MET	B	708	43.770	-13.570	13.497	1.00	19.35	S
ATOM	2129	CE	MET	B	708	44.439	-15.271	13.483	1.00	14.93	C
ATOM	2130	C	MET	B	708	48.674	-12.174	12.299	1.00	18.00	C
ATOM	2131	O	MET	B	708	49.789	-12.726	12.501	1.00	19.56	O
ATOM	2132	N	TYR	B	709	48.316	-11.675	11.129	1.00	18.18	N
ATOM	2133	CA	TYR	B	709	49.206	-11.742	9.981	1.00	18.22	C
ATOM	2134	CB	TYR	B	709	48.600	-11.027	8.799	1.00	18.00	C
ATOM	2135	CG	TYR	B	709	49.392	-11.215	7.533	1.00	20.73	C
ATOM	2136	CD1	TYR	B	709	49.134	-12.285	6.686	1.00	20.65	C
ATOM	2137	CE1	TYR	B	709	49.811	-12.431	5.520	1.00	22.80	C
ATOM	2138	CZ	TYR	B	709	50.778	-11.520	5.187	1.00	23.73	C
ATOM	2139	OH	TYR	B	709	51.492	-11.706	4.041	1.00	23.11	O
ATOM	2140	CE2	TYR	B	709	51.062	-10.456	6.013	1.00	22.99	C
ATOM	2141	CD2	TYR	B	709	50.372	-10.300	7.161	1.00	21.61	C
ATOM	2142	C	TYR	B	709	50.587	-11.163	10.224	1.00	17.84	C
ATOM	2143	O	TYR	B	709	51.559	-11.656	9.676	1.00	17.96	O
ATOM	2144	N	GLY	B	710	50.665	-10.107	11.024	1.00	17.95	N
ATOM	2145	CA	GLY	B	710	51.936	-9.469	11.349	1.00	17.36	C
ATOM	2146	C	GLY	B	710	52.857	-10.280	12.271	1.00	17.08	C
ATOM	2147	O	GLY	B	710	53.937	-10.643	11.848	1.00	18.01	O
ATOM	2148	N	ILE	B	711	52.444	-10.585	13.493	1.00	16.32	N
ATOM	2149	CA	ILE	B	711	53.288	-11.312	14.417	1.00	16.83	C
ATOM	2150	CB	ILE	B	711	52.598	-11.494	15.796	1.00	15.62	C
ATOM	2151	CG1	ILE	B	711	53.286	-10.673	16.876	1.00	17.22	C
ATOM	2152	CD1	ILE	B	711	53.453	-9.239	16.632	1.00	18.82	C
ATOM	2153	CG2	ILE	B	711	52.745	-12.930	16.319	1.00	13.88	C
ATOM	2154	C	ILE	B	711	53.705	-12.666	13.783	1.00	18.91	C
ATOM	2155	O	ILE	B	711	54.827	-13.122	13.926	1.00	17.41	O
ATOM	2156	N	CYS	B	712	52.808	-13.303	13.049	1.00	20.88	N
ATOM	2157	CA	CYS	B	712	53.214	-14.544	12.455	1.00	23.68	C
ATOM	2158	CB	CYS	B	712	52.091	-15.179	11.615	1.00	23.93	C
ATOM	2159	SG	CYS	B	712	50.569	-15.723	12.496	1.00	26.62	S
ATOM	2160	C	CYS	B	712	54.430	-14.237	11.571	1.00	25.43	C
ATOM	2161	O	CYS	B	712	55.390	-15.029	11.516	1.00	25.92	O
ATOM	2162	N	LYS	B	713	54.392	-13.097	10.875	1.00	26.01	N
ATOM	2163	CA	LYS	B	713	55.467	-12.746	9.970	1.00	27.09	C

ATOM	2164	CB	LYS	B	713	55.171	-11.436	9.272	1.00	27.73	C
ATOM	2165	CG	LYS	B	713	54.261	-11.607	8.055	1.00	31.65	C
ATOM	2166	CD	LYS	B	713	54.847	-12.565	7.008	1.00	35.08	C
ATOM	2167	CE	LYS	B	713	54.103	-12.463	5.640	1.00	37.06	C
ATOM	2168	NZ	LYS	B	713	54.896	-13.092	4.488	1.00	37.63	N
ATOM	2169	C	LYS	B	713	56.825	-12.677	10.631	1.00	26.49	C
ATOM	2170	O	LYS	B	713	57.790	-13.241	10.157	1.00	25.93	O
ATOM	2171	N	VAL	B	714	56.900	-11.968	11.736	1.00	26.93	N
ATOM	2172	CA	VAL	B	714	58.181	-11.816	12.437	1.00	26.50	C
ATOM	2173	CB	VAL	B	714	58.141	-10.659	13.427	1.00	26.43	C
ATOM	2174	CG1	VAL	B	714	58.139	-9.365	12.651	1.00	27.09	C
ATOM	2175	CG2	VAL	B	714	56.913	-10.776	14.334	1.00	23.75	C
ATOM	2176	C	VAL	B	714	58.631	-13.072	13.160	1.00	26.16	C
ATOM	2177	O	VAL	B	714	59.795	-13.206	13.464	1.00	26.08	O
ATOM	2178	N	LYS	B	715	57.697	-13.978	13.431	1.00	26.17	N
ATOM	2179	CA	LYS	B	715	58.000	-15.241	14.067	1.00	26.40	C
ATOM	2180	CB	LYS	B	715	56.935	-15.601	15.080	1.00	25.70	C
ATOM	2181	CG	LYS	B	715	56.793	-14.644	16.220	1.00	23.21	C
ATOM	2182	CD	LYS	B	715	57.950	-14.735	17.093	1.00	22.85	C
ATOM	2183	CE	LYS	B	715	57.613	-14.356	18.501	1.00	21.73	C
ATOM	2184	NZ	LYS	B	715	58.799	-14.669	19.392	1.00	20.20	N
ATOM	2185	C	LYS	B	715	58.099	-16.343	13.008	1.00	28.00	C
ATOM	2186	O	LYS	B	715	58.119	-17.523	13.325	1.00	27.94	O
ATOM	2187	N	ASN	B	716	58.164	-15.941	11.749	1.00	29.90	N
ATOM	2188	CA	ASN	B	716	58.255	-16.882	10.639	1.00	32.18	C
ATOM	2189	CB	ASN	B	716	59.663	-17.488	10.599	1.00	33.07	C
ATOM	2190	CG	ASN	B	716	60.627	-16.647	9.764	1.00	34.01	C
ATOM	2191	OD1	ASN	B	716	61.153	-15.622	10.234	1.00	36.77	O
ATOM	2192	ND2	ASN	B	716	60.847	-17.067	8.516	1.00	30.24	N
ATOM	2193	C	ASN	B	716	57.185	-17.991	10.504	1.00	32.52	C
ATOM	2194	O	ASN	B	716	57.395	-18.965	9.773	1.00	32.68	O
ATOM	2195	N	ILE	B	717	56.060	-17.846	11.204	1.00	32.92	N
ATOM	2196	CA	ILE	B	717	54.983	-18.826	11.142	1.00	32.59	C
ATOM	2197	CB	ILE	B	717	54.031	-18.641	12.311	1.00	32.11	C
ATOM	2198	CG1	ILE	B	717	54.799	-18.778	13.620	1.00	32.42	C
ATOM	2199	CD1	ILE	B	717	55.411	-20.122	13.859	1.00	31.30	C
ATOM	2200	CG2	ILE	B	717	52.865	-19.624	12.222	1.00	31.23	C
ATOM	2201	C	ILE	B	717	54.251	-18.581	9.860	1.00	33.04	C

ATOM	2202	O	ILE	B	717	53.776	-17.477	9.616	1.00	34.05	O
ATOM	2203	N	ASP	B	718	54.148	-19.604	9.035	1.00	33.06	N
ATOM	2204	CA	ASP	B	718	53.501	-19.452	7.739	1.00	33.60	C
ATOM	2205	CB	ASP	B	718	53.906	-20.614	6.831	1.00	33.73	C
ATOM	2206	CG	ASP	B	718	53.353	-20.482	5.434	1.00	34.30	C
ATOM	2207	OD1	ASP	B	718	53.839	-19.601	4.661	1.00	32.07	O
ATOM	2208	OD2	ASP	B	718	52.432	-21.237	5.035	1.00	33.96	O
ATOM	2209	C	ASP	B	718	51.974	-19.329	7.795	1.00	33.35	C
ATOM	2210	O	ASP	B	718	51.249	-20.326	7.935	1.00	34.12	O
ATOM	2211	N	LEU	B	719	51.469	-18.114	7.672	1.00	32.76	N
ATOM	2212	CA	LEU	B	719	50.012	-17.908	7.748	1.00	32.36	C
ATOM	2213	CB	LEU	B	719	49.590	-17.409	9.138	1.00	32.31	C
ATOM	2214	CG	LEU	B	719	48.096	-17.110	9.353	1.00	33.01	C
ATOM	2215	CD1	LEU	B	719	47.220	-18.253	8.871	1.00	31.76	C
ATOM	2216	CD2	LEU	B	719	47.761	-16.776	10.820	1.00	32.06	C
ATOM	2217	C	LEU	B	719	49.586	-16.934	6.682	1.00	31.40	C
ATOM	2218	O	LEU	B	719	49.865	-15.743	6.764	1.00	30.98	O
ATOM	2219	N	LYS	B	720	48.937	-17.454	5.664	1.00	30.94	N
ATOM	2220	CA	LYS	B	720	48.521	-16.604	4.573	1.00	31.42	C
ATOM	2221	CB	LYS	B	720	48.380	-17.419	3.278	1.00	31.88	C
ATOM	2222	CG	LYS	B	720	49.634	-18.216	2.944	1.00	33.94	C
ATOM	2223	CD	LYS	B	720	49.478	-19.008	1.649	1.00	37.89	C
ATOM	2224	CE	LYS	B	720	49.501	-18.082	0.379	1.00	39.26	C
ATOM	2225	NZ	LYS	B	720	49.418	-18.855	-0.944	1.00	38.62	N
ATOM	2226	C	LYS	B	720	47.223	-15.858	4.896	1.00	30.27	C
ATOM	2227	O	LYS	B	720	46.347	-16.374	5.592	1.00	30.09	O
ATOM	2228	N	PHE	B	721	47.117	-14.644	4.368	1.00	29.04	N
ATOM	2229	CA	PHE	B	721	45.957	-13.801	4.578	1.00	28.05	C
ATOM	2230	CB	PHE	B	721	46.162	-12.422	3.958	1.00	28.24	C
ATOM	2231	CG	PHE	B	721	46.005	-11.287	4.948	1.00	29.36	C
ATOM	2232	CD1	PHE	B	721	44.870	-11.178	5.715	1.00	31.20	C
ATOM	2233	CE1	PHE	B	721	44.728	-10.147	6.625	1.00	31.53	C
ATOM	2234	CZ	PHE	B	721	45.750	-9.238	6.792	1.00	30.40	C
ATOM	2235	CE2	PHE	B	721	46.885	-9.353	6.050	1.00	29.38	C
ATOM	2236	CD2	PHE	B	721	47.017	-10.361	5.134	1.00	30.03	C
ATOM	2237	C	PHE	B	721	44.714	-14.443	4.011	1.00	27.24	C
ATOM	2238	O	PHE	B	721	43.614	-14.270	4.532	1.00	27.29	O
ATOM	2239	N	LYS	B	722	44.888	-15.203	2.952	1.00	25.84	N

ATOM	2240	CA	LYS	B	722	43.762	-15.855	2.337	1.00	25.19	C
ATOM	2241	CB	LYS	B	722	44.165	-16.442	0.986	1.00	26.12	C
ATOM	2242	CG	LYS	B	722	43.008	-16.961	0.169	1.00	30.46	C
ATOM	2243	CD	LYS	B	722	43.524	-17.782	-1.015	1.00	35.80	C
ATOM	2244	CE	LYS	B	722	44.265	-19.065	-0.529	1.00	37.91	C
ATOM	2245	NZ	LYS	B	722	43.363	-20.138	-0.003	1.00	36.85	N
ATOM	2246	C	LYS	B	722	43.224	-16.916	3.276	1.00	23.23	C
ATOM	2247	O	LYS	B	722	42.052	-17.236	3.235	1.00	23.64	O
ATOM	2248	N	ILE	B	723	44.086	-17.465	4.117	1.00	21.64	N
ATOM	2249	CA	ILE	B	723	43.670	-18.462	5.090	1.00	20.50	C
ATOM	2250	CB	ILE	B	723	44.905	-19.242	5.626	1.00	20.86	C
ATOM	2251	CG1	ILE	B	723	45.479	-20.194	4.560	1.00	22.30	C
ATOM	2252	CD1	ILE	B	723	44.530	-21.368	4.187	1.00	25.70	C
ATOM	2253	CG2	ILE	B	723	44.556	-20.036	6.895	1.00	18.10	C
ATOM	2254	C	ILE	B	723	42.937	-17.771	6.249	1.00	19.81	C
ATOM	2255	O	ILE	B	723	41.997	-18.301	6.822	1.00	20.17	O
ATOM	2256	N	ILE	B	724	43.384	-16.581	6.600	1.00	17.88	N
ATOM	2257	CA	ILE	B	724	42.789	-15.874	7.676	1.00	16.10	C
ATOM	2258	CB	ILE	B	724	43.685	-14.687	8.034	1.00	16.51	C
ATOM	2259	CG1	ILE	B	724	45.116	-15.191	8.240	1.00	13.98	C
ATOM	2260	CD1	ILE	B	724	46.054	-14.177	8.828	1.00	13.32	C
ATOM	2261	CG2	ILE	B	724	43.137	-13.949	9.255	1.00	16.09	C
ATOM	2262	C	ILE	B	724	41.407	-15.432	7.288	1.00	15.97	C
ATOM	2263	O	ILE	B	724	40.475	-15.523	8.079	1.00	15.53	O
ATOM	2264	N	VAL	B	725	41.247	-14.975	6.058	1.00	16.45	N
ATOM	2265	CA	VAL	B	725	39.946	-14.483	5.577	1.00	17.58	C
ATOM	2266	CB	VAL	B	725	40.049	-14.015	4.145	1.00	18.51	C
ATOM	2267	CG1	VAL	B	725	38.846	-14.384	3.410	1.00	19.37	C
ATOM	2268	CG2	VAL	B	725	40.339	-12.541	4.079	1.00	20.64	C
ATOM	2269	C	VAL	B	725	38.878	-15.563	5.615	1.00	17.09	C
ATOM	2270	O	VAL	B	725	37.783	-15.368	6.169	1.00	17.94	O
ATOM	2271	N	THR	B	726	39.216	-16.718	5.067	1.00	16.16	N
ATOM	2272	CA	THR	B	726	38.304	-17.865	5.037	1.00	15.43	C
ATOM	2273	CB	THR	B	726	38.983	-19.089	4.332	1.00	15.56	C
ATOM	2274	OG1	THR	B	726	39.725	-18.634	3.194	1.00	15.24	O
ATOM	2275	CG2	THR	B	726	37.963	-19.961	3.682	1.00	14.25	C
ATOM	2276	C	THR	B	726	37.769	-18.254	6.428	1.00	14.32	C
ATOM	2277	O	THR	B	726	36.600	-18.612	6.590	1.00	13.74	O

ATOM	2278	N	ALA	B	727	38.621	-18.208	7.430	1.00	13.02	N
ATOM	2279	CA	ALA	B	727	38.182	-18.547	8.785	1.00	12.57	C
ATOM	2280	CB	ALA	B	727	39.394	-18.653	9.663	1.00	12.86	C
ATOM	2281	C	ALA	B	727	37.235	-17.440	9.331	1.00	12.91	C
ATOM	2282	O	ALA	B	727	36.101	-17.702	9.745	1.00	11.86	O
ATOM	2283	N	TYR	B	728	37.716	-16.195	9.289	1.00	13.37	N
ATOM	2284	CA	TYR	B	728	36.915	-15.040	9.660	1.00	13.34	C
ATOM	2285	CB	TYR	B	728	37.560	-13.739	9.134	1.00	12.87	C
ATOM	2286	CG	TYR	B	728	36.773	-12.497	9.455	1.00	11.24	C
ATOM	2287	CD1	TYR	B	728	36.790	-11.930	10.738	1.00	9.80	C
ATOM	2288	CE1	TYR	B	728	36.061	-10.794	11.018	1.00	5.74	C
ATOM	2289	CZ	TYR	B	728	35.323	-10.222	10.030	1.00	7.00	C
ATOM	2290	OH	TYR	B	728	34.579	-9.074	10.272	1.00	7.47	O
ATOM	2291	CE2	TYR	B	728	35.308	-10.766	8.777	1.00	5.96	C
ATOM	2292	CD2	TYR	B	728	36.036	-11.875	8.493	1.00	7.33	C
ATOM	2293	C	TYR	B	728	35.496	-15.203	9.111	1.00	13.39	C
ATOM	2294	O	TYR	B	728	34.562	-15.001	9.856	1.00	12.47	O
ATOM	2295	N	LYS	B	729	35.355	-15.598	7.831	1.00	13.99	N
ATOM	2296	CA	LYS	B	729	34.034	-15.706	7.199	1.00	15.28	C
ATOM	2297	CB	LYS	B	729	34.085	-16.311	5.783	1.00	14.79	C
ATOM	2298	CG	LYS	B	729	34.768	-15.480	4.748	1.00	18.29	C
ATOM	2299	CD	LYS	B	729	34.356	-15.844	3.278	1.00	21.11	C
ATOM	2300	CE	LYS	B	729	35.021	-17.144	2.752	1.00	25.75	C
ATOM	2301	NZ	LYS	B	729	34.801	-18.458	3.578	1.00	24.25	N
ATOM	2302	C	LYS	B	729	33.100	-16.568	8.043	1.00	15.73	C
ATOM	2303	O	LYS	B	729	31.884	-16.377	7.977	1.00	14.88	O
ATOM	2304	N	ASP	B	730	33.659	-17.558	8.770	1.00	16.21	N
ATOM	2305	CA	ASP	B	730	32.847	-18.411	9.671	1.00	17.14	C
ATOM	2306	CB	ASP	B	730	33.624	-19.640	10.136	1.00	17.31	C
ATOM	2307	CG	ASP	B	730	33.778	-20.688	9.036	1.00	20.23	C
ATOM	2308	OD1	ASP	B	730	32.778	-20.962	8.350	1.00	22.19	O
ATOM	2309	OD2	ASP	B	730	34.856	-21.298	8.810	1.00	20.06	O
ATOM	2310	C	ASP	B	730	32.241	-17.690	10.914	1.00	16.31	C
ATOM	2311	O	ASP	B	730	31.219	-18.118	11.429	1.00	17.05	O
ATOM	2312	N	LEU	B	731	32.844	-16.610	11.392	1.00	14.65	N
ATOM	2313	CA	LEU	B	731	32.243	-15.945	12.522	1.00	15.22	C
ATOM	2314	CB	LEU	B	731	33.125	-14.789	13.052	1.00	14.75	C
ATOM	2315	CG	LEU	B	731	34.636	-15.126	13.196	1.00	13.31	C

ATOM	2316	CD1	LEU	B	731	35.586	-13.937	13.501	1.00	8.91	C
ATOM	2317	CD2	LEU	B	731	34.775	-16.150	14.223	1.00	11.15	C
ATOM	2318	C	LEU	B	731	30.846	-15.507	12.109	1.00	15.53	C
ATOM	2319	O	LEU	B	731	30.649	-15.085	10.986	1.00	15.48	O
ATOM	2320	N	PRO	B	732	29.874	-15.635	13.008	1.00	16.47	N
ATOM	2321	CA	PRO	B	732	28.444	-15.313	12.714	1.00	17.37	C
ATOM	2322	CB	PRO	B	732	27.732	-15.685	14.022	1.00	17.22	C
ATOM	2323	CG	PRO	B	732	28.872	-15.595	15.072	1.00	16.47	C
ATOM	2324	CD	PRO	B	732	30.066	-16.164	14.367	1.00	15.27	C
ATOM	2325	C	PRO	B	732	28.075	-13.853	12.326	1.00	18.51	C
ATOM	2326	O	PRO	B	732	27.003	-13.592	11.762	1.00	17.81	O
ATOM	2327	N	HIS	B	733	28.931	-12.894	12.620	1.00	19.79	N
ATOM	2328	CA	HIS	B	733	28.578	-11.520	12.293	1.00	21.62	C
ATOM	2329	CB	HIS	B	733	28.964	-10.622	13.462	1.00	22.24	C
ATOM	2330	CG	HIS	B	733	30.392	-10.792	13.863	1.00	26.72	C
ATOM	2331	ND1	HIS	B	733	31.403	-9.962	13.400	1.00	31.50	N
ATOM	2332	CE1	HIS	B	733	32.566	-10.387	13.870	1.00	31.30	C
ATOM	2333	NE2	HIS	B	733	32.343	-11.463	14.614	1.00	32.86	N
ATOM	2334	CD2	HIS	B	733	30.998	-11.751	14.608	1.00	28.05	C
ATOM	2335	C	HIS	B	733	29.366	-11.070	11.077	1.00	21.53	C
ATOM	2336	O	HIS	B	733	29.161	-9.967	10.568	1.00	22.67	O
ATOM	2337	N	ALA	B	734	30.276	-11.924	10.626	1.00	20.57	N
ATOM	2338	CA	ALA	B	734	31.179	-11.610	9.525	1.00	19.72	C
ATOM	2339	CB	ALA	B	734	32.132	-12.798	9.274	1.00	19.49	C
ATOM	2340	C	ALA	B	734	30.555	-11.198	8.210	1.00	18.53	C
ATOM	2341	O	ALA	B	734	29.738	-11.898	7.666	1.00	18.10	O
ATOM	2342	N	VAL	B	735	31.036	-10.096	7.676	1.00	18.27	N
ATOM	2343	CA	VAL	B	735	30.646	-9.624	6.357	1.00	18.38	C
ATOM	2344	CB	VAL	B	735	30.027	-8.272	6.466	1.00	17.76	C
ATOM	2345	CG1	VAL	B	735	29.805	-7.694	5.093	1.00	19.37	C
ATOM	2346	CG2	VAL	B	735	28.741	-8.437	7.141	1.00	17.16	C
ATOM	2347	C	VAL	B	735	31.832	-9.562	5.428	1.00	18.15	C
ATOM	2348	O	VAL	B	735	32.839	-8.983	5.751	1.00	18.71	O
ATOM	2349	N	GLN	B	736	31.712	-10.129	4.245	1.00	19.52	N
ATOM	2350	CA	GLN	B	736	32.851	-10.140	3.292	1.00	20.24	C
ATOM	2351	CB	GLN	B	736	32.435	-10.691	1.937	1.00	21.49	C
ATOM	2352	CG	GLN	B	736	32.023	-12.190	1.994	1.00	26.42	C
ATOM	2353	CD	GLN	B	736	32.035	-12.854	0.580	1.00	30.92	C

ATOM	2354	OE1	GLN	B	736	33.109	-13.248	0.047	1.00	30.86	O
ATOM	2355	NE2	GLN	B	736	30.851	-12.949	-0.024	1.00	30.08	N
ATOM	2356	C	GLN	B	736	33.517	-8.799	3.100	1.00	18.33	C
ATOM	2357	O	GLN	B	736	34.771	-8.694	3.090	1.00	19.47	O
ATOM	2358	N	GLU	B	737	32.672	-7.793	2.972	1.00	15.56	N
ATOM	2359	CA	GLU	B	737	33.095	-6.424	2.769	1.00	14.71	C
ATOM	2360	CB	GLU	B	737	31.857	-5.518	2.763	1.00	13.93	C
ATOM	2361	CG	GLU	B	737	32.132	-4.035	2.789	1.00	20.16	C
ATOM	2362	CD	GLU	B	737	30.887	-3.181	3.145	1.00	29.64	C
ATOM	2363	OE1	GLU	B	737	30.162	-3.607	4.089	1.00	34.03	O
ATOM	2364	OE2	GLU	B	737	30.615	-2.096	2.518	1.00	27.73	O
ATOM	2365	C	GLU	B	737	34.206	-5.959	3.756	1.00	13.09	C
ATOM	2366	O	GLU	B	737	35.063	-5.162	3.389	1.00	13.18	O
ATOM	2367	N	THR	B	738	34.224	-6.472	4.984	1.00	11.57	N
ATOM	2368	CA	THR	B	738	35.257	-6.065	5.951	1.00	10.08	C
ATOM	2369	CB	THR	B	738	34.999	-6.653	7.332	1.00	8.74	C
ATOM	2370	OG1	THR	B	738	33.648	-6.403	7.711	1.00	9.41	O
ATOM	2371	CG2	THR	B	738	35.757	-5.946	8.356	1.00	2.00	C
ATOM	2372	C	THR	B	738	36.728	-6.349	5.527	1.00	10.98	C
ATOM	2373	O	THR	B	738	37.616	-5.661	5.995	1.00	9.61	O
ATOM	2374	N	PHE	B	739	36.976	-7.314	4.634	1.00	12.04	N
ATOM	2375	CA	PHE	B	739	38.338	-7.514	4.109	1.00	13.84	C
ATOM	2376	CB	PHE	B	739	38.926	-8.893	4.455	1.00	13.62	C
ATOM	2377	CG	PHE	B	739	38.107	-10.029	3.986	1.00	14.17	C
ATOM	2378	CD1	PHE	B	739	38.063	-10.348	2.633	1.00	14.68	C
ATOM	2379	CE1	PHE	B	739	37.279	-11.414	2.175	1.00	12.99	C
ATOM	2380	CZ	PHE	B	739	36.511	-12.157	3.098	1.00	11.66	C
ATOM	2381	CE2	PHE	B	739	36.550	-11.832	4.439	1.00	12.82	C
ATOM	2382	CD2	PHE	B	739	37.348	-10.775	4.879	1.00	12.84	C
ATOM	2383	C	PHE	B	739	38.449	-7.259	2.590	1.00	15.45	C
ATOM	2384	O	PHE	B	739	39.537	-7.256	2.013	1.00	16.07	O
ATOM	2385	N	LYS	B	740	37.338	-7.031	1.912	1.00	16.42	N
ATOM	2386	CA	LYS	B	740	37.424	-6.723	0.479	1.00	16.15	C
ATOM	2387	CB	LYS	B	740	36.213	-7.289	-0.258	1.00	17.06	C
ATOM	2388	CG	LYS	B	740	36.071	-8.841	-0.313	1.00	18.60	C
ATOM	2389	CD	LYS	B	740	35.364	-9.271	-1.631	1.00	17.32	C
ATOM	2390	CE	LYS	B	740	34.757	-10.655	-1.542	1.00	22.65	C
ATOM	2391	NZ	LYS	B	740	35.750	-11.740	-1.288	1.00	26.48	N

ATOM	2392	C	LYS	B	740	37.470	-5.213	0.201	1.00	15.61	C
ATOM	2393	O	LYS	B	740	37.968	-4.795	-0.822	1.00	14.70	O
ATOM	2394	N	ARG	B	741	36.920	-4.416	1.127	1.00	15.05	N
ATOM	2395	CA	ARG	B	741	36.797	-2.962	0.995	1.00	14.19	C
ATOM	2396	CB	ARG	B	741	35.330	-2.620	0.730	1.00	14.64	C
ATOM	2397	CG	ARG	B	741	35.008	-1.179	0.421	1.00	16.18	C
ATOM	2398	CD	ARG	B	741	33.588	-0.966	-0.148	1.00	24.70	C
ATOM	2399	NE	ARG	B	741	33.531	0.033	-1.252	1.00	25.41	N
ATOM	2400	CZ	ARG	B	741	33.785	1.342	-1.084	1.00	26.65	C
ATOM	2401	NH1	ARG	B	741	34.096	1.807	0.123	1.00	25.62	N
ATOM	2402	NH2	ARG	B	741	33.733	2.193	-2.102	1.00	25.67	N
ATOM	2403	C	ARG	B	741	37.245	-2.300	2.291	1.00	13.80	C
ATOM	2404	O	ARG	B	741	36.469	-2.118	3.199	1.00	12.81	O
ATOM	2405	N	VAL	B	742	38.519	-1.966	2.379	1.00	13.97	N
ATOM	2406	CA	VAL	B	742	39.089	-1.379	3.586	1.00	14.00	C
ATOM	2407	CB	VAL	B	742	40.197	-2.276	4.165	1.00	14.78	C
ATOM	2408	CG1	VAL	B	742	40.864	-1.627	5.411	1.00	12.67	C
ATOM	2409	CG2	VAL	B	742	39.671	-3.683	4.413	1.00	13.17	C
ATOM	2410	C	VAL	B	742	39.698	-0.039	3.193	1.00	13.99	C
ATOM	2411	O	VAL	B	742	40.175	0.101	2.069	1.00	13.44	O
ATOM	2412	N	LEU	B	743	39.640	0.928	4.096	1.00	14.08	N
ATOM	2413	CA	LEU	B	743	40.118	2.281	3.834	1.00	16.23	C
ATOM	2414	CB	LEU	B	743	39.695	3.196	4.950	1.00	16.17	C
ATOM	2415	CG	LEU	B	743	39.291	4.624	4.687	1.00	17.47	C
ATOM	2416	CD1	LEU	B	743	39.320	5.415	5.988	1.00	16.65	C
ATOM	2417	CD2	LEU	B	743	40.177	5.284	3.687	1.00	19.65	C
ATOM	2418	C	LEU	B	743	41.622	2.365	3.695	1.00	17.49	C
ATOM	2419	O	LEU	B	743	42.360	1.710	4.400	1.00	17.60	O
ATOM	2420	N	ILE	B	744	42.072	3.160	2.744	1.00	20.53	N
ATOM	2421	CA	ILE	B	744	43.492	3.338	2.533	1.00	23.74	C
ATOM	2422	CB	ILE	B	744	43.902	2.930	1.102	1.00	24.04	C
ATOM	2423	CG1	ILE	B	744	43.379	1.514	0.756	1.00	22.67	C
ATOM	2424	CD1	ILE	B	744	43.896	0.426	1.560	1.00	19.74	C
ATOM	2425	CG2	ILE	B	744	45.405	2.990	0.952	1.00	23.62	C
ATOM	2426	C	ILE	B	744	43.982	4.733	2.819	1.00	25.89	C
ATOM	2427	O	ILE	B	744	44.797	4.898	3.691	1.00	26.76	O
ATOM	2428	N	LYS	B	745	43.493	5.737	2.100	1.00	28.94	N
ATOM	2429	CA	LYS	B	745	44.043	7.102	2.253	1.00	31.98	C

ATOM	2430	CB	LYS	B	745	44.911	7.474	1.035	1.00	31.99	C
ATOM	2431	CG	LYS	B	745	46.346	6.997	1.095	1.00	33.87	C
ATOM	2432	CD	LYS	B	745	46.918	6.683	-0.307	1.00	35.93	C
ATOM	2433	CE	LYS	B	745	47.283	7.943	-1.086	1.00	33.52	C
ATOM	2434	NZ	LYS	B	745	46.120	8.507	-1.826	1.00	32.74	N
ATOM	2435	C	LYS	B	745	43.011	8.218	2.510	1.00	33.73	C
ATOM	2436	O	LYS	B	745	43.033	8.889	3.574	1.00	35.26	O
ATOM	2437	N	GLU	B	746	42.125	8.457	1.542	1.00	34.28	N
ATOM	2438	CA	GLU	B	746	41.094	9.456	1.767	1.00	35.03	C
ATOM	2439	CB	GLU	B	746	41.370	10.733	0.995	1.00	35.68	C
ATOM	2440	CG	GLU	B	746	41.647	10.472	-0.457	1.00	39.53	C
ATOM	2441	CD	GLU	B	746	42.782	9.502	-0.614	1.00	42.55	C
ATOM	2442	OE1	GLU	B	746	43.920	9.880	-0.281	1.00	42.51	O
ATOM	2443	OE2	GLU	B	746	42.519	8.364	-1.034	1.00	47.78	O
ATOM	2444	C	GLU	B	746	39.726	8.925	1.439	1.00	34.47	C
ATOM	2445	O	GLU	B	746	38.844	8.974	2.266	1.00	36.86	O
ATOM	2446	N	GLU	B	747	39.526	8.424	0.234	1.00	33.35	N
ATOM	2447	CA	GLU	B	747	38.245	7.839	-0.115	1.00	31.94	C
ATOM	2448	CB	GLU	B	747	37.426	8.821	-0.936	1.00	32.95	C
ATOM	2449	CG	GLU	B	747	37.090	10.125	-0.212	1.00	36.33	C
ATOM	2450	CD	GLU	B	747	35.781	10.735	-0.705	1.00	39.89	C
ATOM	2451	OE1	GLU	B	747	34.720	10.153	-0.373	1.00	39.59	O
ATOM	2452	OE2	GLU	B	747	35.812	11.772	-1.431	1.00	40.99	O
ATOM	2453	C	GLU	B	747	38.504	6.586	-0.928	1.00	30.15	C
ATOM	2454	O	GLU	B	747	37.614	6.091	-1.625	1.00	29.18	O
ATOM	2455	N	GLU	B	748	39.747	6.109	-0.820	1.00	28.29	N
ATOM	2456	CA	GLU	B	748	40.251	4.934	-1.509	1.00	27.13	C
ATOM	2457	CB	GLU	B	748	41.666	5.225	-2.007	1.00	27.78	C
ATOM	2458	CG	GLU	B	748	42.369	4.026	-2.600	1.00	31.92	C
ATOM	2459	CD	GLU	B	748	41.560	3.391	-3.728	1.00	39.42	C
ATOM	2460	OE1	GLU	B	748	40.892	4.135	-4.511	1.00	41.77	O
ATOM	2461	OE2	GLU	B	748	41.576	2.138	-3.828	1.00	41.89	O
ATOM	2462	C	GLU	B	748	40.192	3.607	-0.701	1.00	25.04	C
ATOM	2463	O	GLU	B	748	40.724	3.480	0.411	1.00	23.53	O
ATOM	2464	N	TYR	B	749	39.506	2.621	-1.270	1.00	23.64	N
ATOM	2465	CA	TYR	B	749	39.390	1.305	-0.645	1.00	21.89	C
ATOM	2466	CB	TYR	B	749	37.939	1.027	-0.350	1.00	21.59	C
ATOM	2467	CG	TYR	B	749	37.363	1.979	0.662	1.00	19.85	C

ATOM	2468	CD1	TYR	B	749	37.125	3.290	0.327	1.00	17.50	C
ATOM	2469	CE1	TYR	B	749	36.596	4.167	1.231	1.00	19.14	C
ATOM	2470	CZ	TYR	B	749	36.300	3.745	2.506	1.00	19.16	C
ATOM	2471	OH	TYR	B	749	35.764	4.657	3.419	1.00	18.64	O
ATOM	2472	CE2	TYR	B	749	36.536	2.427	2.857	1.00	19.01	C
ATOM	2473	CD2	TYR	B	749	37.063	1.563	1.946	1.00	17.38	C
ATOM	2474	C	TYR	B	749	39.964	0.192	-1.504	1.00	20.89	C
ATOM	2475	O	TYR	B	749	39.916	0.259	-2.716	1.00	21.97	O
ATOM	2476	N	ASP	B	750	40.494	-0.837	-0.866	1.00	20.13	N
ATOM	2477	CA	ASP	B	750	41.111	-1.970	-1.538	1.00	18.82	C
ATOM	2478	CB	ASP	B	750	42.567	-1.679	-1.874	1.00	19.07	C
ATOM	2479	CG	ASP	B	750	42.941	-2.117	-3.312	1.00	20.57	C
ATOM	2480	OD1	ASP	B	750	42.687	-3.314	-3.677	1.00	15.59	O
ATOM	2481	OD2	ASP	B	750	43.496	-1.299	-4.114	1.00	20.85	O
ATOM	2482	C	ASP	B	750	41.067	-3.110	-0.580	1.00	17.86	C
ATOM	2483	O	ASP	B	750	40.606	-2.927	0.545	1.00	18.20	O
ATOM	2484	N	SER	B	751	41.534	-4.277	-1.023	1.00	16.66	N
ATOM	2485	CA	SER	B	751	41.594	-5.478	-0.198	1.00	15.69	C
ATOM	2486	CB	SER	B	751	42.277	-6.578	-0.976	1.00	14.91	C
ATOM	2487	OG	SER	B	751	43.683	-6.392	-0.953	1.00	15.07	O
ATOM	2488	C	SER	B	751	42.349	-5.264	1.138	1.00	15.52	C
ATOM	2489	O	SER	B	751	43.138	-4.346	1.310	1.00	15.02	O
ATOM	2490	N	ILE	B	752	42.142	-6.147	2.083	1.00	15.22	N
ATOM	2491	CA	ILE	B	752	42.790	-5.968	3.367	1.00	15.33	C
ATOM	2492	CB	ILE	B	752	42.236	-6.937	4.387	1.00	14.48	C
ATOM	2493	CG1	ILE	B	752	42.606	-6.495	5.805	1.00	15.87	C
ATOM	2494	CD1	ILE	B	752	41.941	-7.320	6.917	1.00	12.60	C
ATOM	2495	CG2	ILE	B	752	42.760	-8.248	4.108	1.00	14.29	C
ATOM	2496	C	ILE	B	752	44.295	-6.089	3.284	1.00	15.94	C
ATOM	2497	O	ILE	B	752	44.984	-5.642	4.209	1.00	16.82	O
ATOM	2498	N	ILE	B	753	44.803	-6.656	2.186	1.00	15.32	N
ATOM	2499	CA	ILE	B	753	46.219	-6.847	2.011	1.00	15.05	C
ATOM	2500	CB	ILE	B	753	46.481	-7.795	0.834	1.00	16.49	C
ATOM	2501	CG1	ILE	B	753	46.016	-9.193	1.137	1.00	17.73	C
ATOM	2502	CD1	ILE	B	753	45.975	-10.051	-0.111	1.00	17.48	C
ATOM	2503	CG2	ILE	B	753	47.962	-7.928	0.502	1.00	17.13	C
ATOM	2504	C	ILE	B	753	46.830	-5.512	1.672	1.00	14.92	C
ATOM	2505	O	ILE	B	753	47.876	-5.155	2.189	1.00	15.50	O

ATOM	2506	N	VAL	B	754	46.222	-4.772	0.756	1.00	14.19	N
ATOM	2507	CA	VAL	B	754	46.811	-3.490	0.387	1.00	13.27	C
ATOM	2508	CB	VAL	B	754	45.977	-2.757	-0.669	1.00	13.73	C
ATOM	2509	CG1	VAL	B	754	46.516	-1.366	-0.960	1.00	13.78	C
ATOM	2510	CG2	VAL	B	754	45.829	-3.593	-1.938	1.00	13.40	C
ATOM	2511	C	VAL	B	754	46.863	-2.657	1.656	1.00	13.15	C
ATOM	2512	O	VAL	B	754	47.807	-1.884	1.862	1.00	12.76	O
ATOM	2513	N	PHE	B	755	45.863	-2.832	2.528	1.00	12.25	N
ATOM	2514	CA	PHE	B	755	45.849	-2.081	3.763	1.00	11.74	C
ATOM	2515	CB	PHE	B	755	44.564	-2.286	4.554	1.00	12.24	C
ATOM	2516	CG	PHE	B	755	44.591	-1.641	5.917	1.00	9.65	C
ATOM	2517	CD1	PHE	B	755	44.648	-0.250	6.030	1.00	11.69	C
ATOM	2518	CE1	PHE	B	755	44.710	0.373	7.313	1.00	13.58	C
ATOM	2519	CZ	PHE	B	755	44.678	-0.431	8.444	1.00	12.16	C
ATOM	2520	CE2	PHE	B	755	44.603	-1.833	8.307	1.00	8.49	C
ATOM	2521	CD2	PHE	B	755	44.568	-2.414	7.070	1.00	5.62	C
ATOM	2522	C	PHE	B	755	47.028	-2.440	4.638	1.00	11.89	C
ATOM	2523	O	PHE	B	755	47.725	-1.554	5.142	1.00	10.64	O
ATOM	2524	N	TYR	B	756	47.239	-3.741	4.848	1.00	12.44	N
ATOM	2525	CA	TYR	B	756	48.369	-4.170	5.674	1.00	13.71	C
ATOM	2526	CB	TYR	B	756	48.450	-5.675	5.721	1.00	13.48	C
ATOM	2527	CG	TYR	B	756	49.697	-6.181	6.414	1.00	16.30	C
ATOM	2528	CD1	TYR	B	756	49.792	-6.197	7.793	1.00	16.18	C
ATOM	2529	CE1	TYR	B	756	50.933	-6.683	8.441	1.00	18.26	C
ATOM	2530	CZ	TYR	B	756	52.012	-7.161	7.687	1.00	21.98	C
ATOM	2531	OH	TYR	B	756	53.166	-7.628	8.297	1.00	17.21	O
ATOM	2532	CE2	TYR	B	756	51.935	-7.156	6.293	1.00	20.27	C
ATOM	2533	CD2	TYR	B	756	50.782	-6.674	5.673	1.00	20.75	C
ATOM	2534	C	TYR	B	756	49.688	-3.564	5.123	1.00	14.37	C
ATOM	2535	O	TYR	B	756	50.386	-2.764	5.791	1.00	14.12	O
ATOM	2536	N	ASN	B	757	49.988	-3.880	3.867	1.00	14.19	N
ATOM	2537	CA	ASN	B	757	51.213	-3.374	3.300	1.00	15.33	C
ATOM	2538	CB	ASN	B	757	51.516	-4.070	1.984	1.00	15.54	C
ATOM	2539	CG	ASN	B	757	51.770	-5.537	2.177	1.00	18.19	C
ATOM	2540	OD1	ASN	B	757	52.778	-5.936	2.783	1.00	19.68	O
ATOM	2541	ND2	ASN	B	757	50.851	-6.363	1.680	1.00	20.50	N
ATOM	2542	C	ASN	B	757	51.320	-1.860	3.141	1.00	14.85	C
ATOM	2543	O	ASN	B	757	52.419	-1.337	3.198	1.00	15.14	O

ATOM	2544	N	SER	B	758	50.210	-1.162	2.942	1.00	13.60		N
ATOM	2545	CA	SER	B	758	50.310	0.251	2.646	1.00	13.76		C
ATOM	2546	CB	SER	B	758	49.283	0.667	1.603	1.00	13.54		C
ATOM	2547	OG	SER	B	758	49.507	-0.024	0.387	1.00	15.82		O
ATOM	2548	C	SER	B	758	50.167	1.178	3.823	1.00	14.24		C
ATOM	2549	O	SER	B	758	50.628	2.331	3.727	1.00	14.50		O
ATOM	2550	N	VAL	B	759	49.516	0.701	4.899	1.00	13.20		N
ATOM	2551	CA	VAL	B	759	49.204	1.515	6.035	1.00	12.81		C
ATOM	2552	CB	VAL	B	759	47.751	1.834	6.030	1.00	12.98		C
ATOM	2553	CG1	VAL	B	759	47.457	2.869	7.066	1.00	12.46		C
ATOM	2554	CG2	VAL	B	759	47.378	2.343	4.650	1.00	13.50		C
ATOM	2555	C	VAL	B	759	49.558	0.906	7.375	1.00	14.10		C
ATOM	2556	O	VAL	B	759	50.245	1.528	8.144	1.00	14.24		O
ATOM	2557	N	PHE	B	760	49.113	-0.320	7.641	1.00	14.78		N
ATOM	2558	CA	PHE	B	760	49.305	-0.964	8.916	1.00	15.29		C
ATOM	2559	CB	PHE	B	760	48.569	-2.314	8.884	1.00	15.21		C
ATOM	2560	CG	PHE	B	760	48.414	-2.965	10.234	1.00	14.87		C
ATOM	2561	CD1	PHE	B	760	47.385	-2.591	11.085	1.00	13.04		C
ATOM	2562	CE1	PHE	B	760	47.237	-3.188	12.302	1.00	13.09		C
ATOM	2563	CZ	PHE	B	760	48.118	-4.129	12.712	1.00	13.72		C
ATOM	2564	CE2	PHE	B	760	49.165	-4.488	11.897	1.00	15.35		C
ATOM	2565	CD2	PHE	B	760	49.304	-3.918	10.660	1.00	13.80		C
ATOM	2566	C	PHE	B	760	50.785	-1.162	9.246	1.00	16.61		C
ATOM	2567	O	PHE	B	760	51.333	-0.642	10.217	1.00	16.43		O
ATOM	2568	N	MET	B	761	51.422	-1.954	8.426	1.00	18.47		N
ATOM	2569	CA	MET	B	761	52.791	-2.303	8.631	1.00	21.12		C
ATOM	2570	CB	MET	B	761	53.267	-3.148	7.451	1.00	22.42		C
ATOM	2571	CG	MET	B	761	54.775	-3.092	7.205	1.00	24.52		C
ATOM	2572	SD	MET	B	761	55.033	-4.025	5.779	1.00	32.46		S
ATOM	2573	CE	MET	B	761	55.132	-5.783	6.464	1.00	33.08		C
ATOM	2574	C	MET	B	761	53.689	-1.091	8.816	1.00	21.28		C
ATOM	2575	O	MET	B	761	54.647	-1.132	9.533	1.00	22.18		O
ATOM	2576	N	GLN	B	762	53.381	-0.005	8.159	1.00	22.50		N
ATOM	2577	CA	GLN	B	762	54.223	1.171	8.259	1.00	22.90		C
ATOM	2578	CB	GLN	B	762	53.913	2.123	7.106	1.00	23.18		C
ATOM	2579	CG	GLN	B	762	53.783	1.393	5.714	1.00	27.77		C
ATOM	2580	CD	GLN	B	762	55.041	0.617	5.279	1.00	32.36		C
ATOM	2581	OE1	GLN	B	762	55.947	1.172	4.658	1.00	34.37		O

ATOM	2582	NE2	GLN	B	762	55.071	-0.687	5.585	1.00	36.21	N
ATOM	2583	C	GLN	B	762	54.043	1.853	9.593	1.00	21.95	C
ATOM	2584	O	GLN	B	762	54.985	2.236	10.247	1.00	21.06	O
ATOM	2585	N	ARG	B	763	52.815	2.011	10.012	1.00	21.79	N
ATOM	2586	CA	ARG	B	763	52.622	2.728	11.232	1.00	22.55	C
ATOM	2587	CB	ARG	B	763	51.143	3.037	11.405	1.00	23.18	C
ATOM	2588	CG	ARG	B	763	50.785	3.636	12.785	1.00	27.01	C
ATOM	2589	CD	ARG	B	763	51.197	5.097	12.938	1.00	31.66	C
ATOM	2590	NE	ARG	B	763	50.298	5.888	12.126	1.00	36.41	N
ATOM	2591	CZ	ARG	B	763	49.055	6.188	12.498	1.00	39.77	C
ATOM	2592	NH1	ARG	B	763	48.603	5.780	13.691	1.00	36.61	N
ATOM	2593	NH2	ARG	B	763	48.273	6.913	11.691	1.00	40.01	N
ATOM	2594	C	ARG	B	763	53.158	1.947	12.436	1.00	22.17	C
ATOM	2595	O	ARG	B	763	53.538	2.537	13.438	1.00	19.77	O
ATOM	2596	N	LEU	B	764	53.190	0.617	12.300	1.00	22.80	N
ATOM	2597	CA	LEU	B	764	53.588	-0.269	13.386	1.00	23.24	C
ATOM	2598	CB	LEU	B	764	52.500	-1.301	13.594	1.00	23.48	C
ATOM	2599	CG	LEU	B	764	51.177	-0.718	14.097	1.00	24.36	C
ATOM	2600	CD1	LEU	B	764	50.013	-1.676	13.885	1.00	24.21	C
ATOM	2601	CD2	LEU	B	764	51.348	-0.480	15.529	1.00	24.26	C
ATOM	2602	C	LEU	B	764	54.917	-0.993	13.193	1.00	23.50	C
ATOM	2603	O	LEU	B	764	55.345	-1.716	14.089	1.00	21.69	O
ATOM	2604	N	LYS	B	765	55.556	-0.812	12.032	1.00	24.54	N
ATOM	2605	CA	LYS	B	765	56.800	-1.510	11.719	1.00	26.74	C
ATOM	2606	CB	LYS	B	765	57.462	-0.944	10.464	1.00	26.88	C
ATOM	2607	CG	LYS	B	765	58.915	-1.493	10.240	1.00	28.72	C
ATOM	2608	CD	LYS	B	765	59.559	-1.044	8.915	1.00	31.45	C
ATOM	2609	CE	LYS	B	765	58.982	-1.767	7.693	1.00	34.41	C
ATOM	2610	NZ	LYS	B	765	57.496	-1.689	7.597	1.00	37.61	N
ATOM	2611	C	LYS	B	765	57.796	-1.462	12.879	1.00	28.01	C
ATOM	2612	O	LYS	B	765	58.254	-2.494	13.377	1.00	27.53	O
ATOM	2613	N	THR	B	766	58.126	-0.242	13.273	1.00	29.05	N
ATOM	2614	CA	THR	B	766	58.966	0.013	14.424	1.00	30.88	C
ATOM	2615	CB	THR	B	766	58.821	1.516	14.840	1.00	31.26	C
ATOM	2616	OG1	THR	B	766	59.035	2.348	13.698	1.00	33.49	O
ATOM	2617	CG2	THR	B	766	59.909	1.962	15.802	1.00	30.65	C
ATOM	2618	C	THR	B	766	58.615	-0.872	15.610	1.00	30.99	C
ATOM	2619	O	THR	B	766	59.449	-1.569	16.119	1.00	32.43	O

ATOM	2620	N	ASN	B	767	57.398	-0.804	16.083	1.00	31.61	N
ATOM	2621	CA	ASN	B	767	56.992	-1.570	17.232	1.00	33.54	C
ATOM	2622	CB	ASN	B	767	55.652	-1.023	17.768	1.00	33.93	C
ATOM	2623	CG	ASN	B	767	55.048	-1.892	18.837	1.00	36.39	C
ATOM	2624	OD1	ASN	B	767	54.504	-2.945	18.545	1.00	39.39	O
ATOM	2625	ND2	ASN	B	767	55.142	-1.456	20.094	1.00	40.65	N
ATOM	2626	C	ASN	B	767	56.926	-3.092	16.985	1.00	34.59	C
ATOM	2627	O	ASN	B	767	57.394	-3.895	17.816	1.00	34.71	O
ATOM	2628	N	ILE	B	768	56.354	-3.511	15.863	1.00	35.47	N
ATOM	2629	CA	ILE	B	768	56.239	-4.940	15.625	1.00	36.32	C
ATOM	2630	CB	ILE	B	768	55.621	-5.237	14.268	1.00	36.49	C
ATOM	2631	CG1	ILE	B	768	54.105	-4.966	14.309	1.00	35.72	C
ATOM	2632	CD1	ILE	B	768	53.429	-5.168	12.981	1.00	35.45	C
ATOM	2633	CG2	ILE	B	768	55.950	-6.683	13.834	1.00	34.18	C
ATOM	2634	C	ILE	B	768	57.592	-5.577	15.698	1.00	37.63	C
ATOM	2635	O	ILE	B	768	57.694	-6.786	15.923	1.00	38.19	O
ATOM	2636	N	LEU	B	769	58.626	-4.764	15.505	1.00	38.55	N
ATOM	2637	CA	LEU	B	769	59.996	-5.257	15.523	1.00	40.19	C
ATOM	2638	CB	LEU	B	769	60.996	-4.186	15.082	1.00	40.99	C
ATOM	2639	CG	LEU	B	769	61.863	-4.615	13.896	1.00	42.49	C
ATOM	2640	CD1	LEU	B	769	62.460	-5.984	14.251	1.00	45.30	C
ATOM	2641	CD2	LEU	B	769	61.061	-4.723	12.578	1.00	42.90	C
ATOM	2642	C	LEU	B	769	60.375	-5.753	16.890	1.00	40.93	C
ATOM	2643	O	LEU	B	769	61.022	-6.789	16.999	1.00	41.56	O
ATOM	2644	N	GLN	B	770	59.987	-5.024	17.936	1.00	41.51	N
ATOM	2645	CA	GLN	B	770	60.285	-5.473	19.304	1.00	41.74	C
ATOM	2646	CB	GLN	B	770	59.366	-4.794	20.343	1.00	41.53	C
ATOM	2647	CG	GLN	B	770	59.450	-5.418	21.762	1.00	42.43	C
ATOM	2648	CD	GLN	B	770	58.133	-5.425	22.587	1.00	42.74	C
ATOM	2649	OE1	GLN	B	770	58.064	-6.041	23.668	1.00	41.16	O
ATOM	2650	NE2	GLN	B	770	57.116	-4.740	22.090	1.00	43.74	N
ATOM	2651	C	GLN	B	770	60.125	-7.004	19.380	1.00	41.82	C
ATOM	2652	O	GLN	B	770	61.077	-7.747	19.610	1.00	41.81	O
ATOM	2653	N	TYR	B	771	58.911	-7.467	19.144	1.00	42.24	N
ATOM	2654	CA	TYR	B	771	58.610	-8.888	19.229	1.00	42.97	C
ATOM	2655	CB	TYR	B	771	57.180	-9.140	18.775	1.00	41.87	C
ATOM	2656	CG	TYR	B	771	56.175	-8.189	19.354	1.00	38.45	C
ATOM	2657	CD1	TYR	B	771	55.729	-8.307	20.662	1.00	37.30	C

ATOM	2658	CE1	TYR	B	771	54.776	-7.426	21.169	1.00	35.23	C
ATOM	2659	CZ	TYR	B	771	54.263	-6.431	20.343	1.00	34.31	C
ATOM	2660	OH	TYR	B	771	53.309	-5.491	20.752	1.00	34.71	O
ATOM	2661	CE2	TYR	B	771	54.703	-6.332	19.061	1.00	33.76	C
ATOM	2662	CD2	TYR	B	771	55.641	-7.191	18.576	1.00	35.17	C
ATOM	2663	C	TYR	B	771	59.572	-9.775	18.441	1.00	44.15	C
ATOM	2664	O	TYR	B	771	59.703	-10.968	18.720	1.00	43.36	O
ATOM	2665	N	ALA	B	772	60.235	-9.181	17.454	1.00	46.14	N
ATOM	2666	CA	ALA	B	772	61.159	-9.932	16.620	1.00	48.39	C
ATOM	2667	CB	ALA	B	772	61.590	-9.113	15.432	1.00	48.34	C
ATOM	2668	C	ALA	B	772	62.368	-10.356	17.425	1.00	50.30	C
ATOM	2669	O	ALA	B	772	62.956	-11.413	17.175	1.00	50.02	O
ATOM	2670	N	SER	B	773	62.746	-9.510	18.383	1.00	52.64	N
ATOM	2671	CA	SER	B	773	63.884	-9.794	19.238	1.00	54.66	C
ATOM	2672	CB	SER	B	773	64.021	-8.723	20.320	1.00	54.48	C
ATOM	2673	OG	SER	B	773	65.106	-9.024	21.187	1.00	55.08	O
ATOM	2674	C	SER	B	773	63.691	-11.173	19.879	1.00	56.17	C
ATOM	2675	O	SER	B	773	62.634	-11.447	20.455	1.00	56.55	O
ATOM	2676	N	THR	B	774	64.709	-12.031	19.768	1.00	57.80	N
ATOM	2677	CA	THR	B	774	64.694	-13.397	20.328	1.00	59.18	C
ATOM	2678	CB	THR	B	774	65.990	-14.164	19.901	1.00	59.51	C
ATOM	2679	OG1	THR	B	774	67.155	-13.432	20.324	1.00	60.23	O
ATOM	2680	CG2	THR	B	774	66.138	-14.219	18.355	1.00	59.89	C
ATOM	2681	C	THR	B	774	64.527	-13.436	21.875	1.00	59.52	C
ATOM	2682	O	THR	B	774	64.836	-14.440	22.533	1.00	59.47	O
ATOM	2683	N	ARG	B	775	64.043	-12.330	22.433	1.00	59.58	N
ATOM	2684	CA	ARG	B	775	63.800	-12.203	23.861	1.00	59.55	C
ATOM	2685	CB	ARG	B	775	64.540	-10.968	24.393	1.00	59.96	C
ATOM	2686	CG	ARG	B	775	64.053	-9.623	23.789	1.00	60.09	C
ATOM	2687	CD	ARG	B	775	64.791	-8.402	24.311	1.00	59.27	C
ATOM	2688	NE	ARG	B	775	64.233	-7.147	23.810	1.00	58.26	N
ATOM	2689	CZ	ARG	B	775	63.016	-6.685	24.091	1.00	57.54	C
ATOM	2690	NH1	ARG	B	775	62.186	-7.364	24.871	1.00	56.28	N
ATOM	2691	NH2	ARG	B	775	62.618	-5.532	23.577	1.00	57.23	N
ATOM	2692	C	ARG	B	775	62.283	-12.077	24.117	1.00	59.35	C
ATOM	2693	O	ARG	B	775	61.559	-11.452	23.327	1.00	59.00	O
ATOM	2694	N	PRO	B	776	61.799	-12.663	25.217	1.00	59.19	N
ATOM	2695	CA	PRO	B	776	60.358	-12.614	25.546	1.00	58.52	C

ATOM	2696	CB	PRO	B	776	60.263	-13.471	26.817	1.00	58.69	C
ATOM	2697	CG	PRO	B	776	61.659	-13.372	27.413	1.00	59.27	C
ATOM	2698	CD	PRO	B	776	62.577	-13.431	26.219	1.00	59.00	C
ATOM	2699	C	PRO	B	776	59.846	-11.173	25.804	1.00	57.74	C
ATOM	2700	O	PRO	B	776	60.560	-10.337	26.404	1.00	57.92	O
ATOM	2701	N	PRO	B	777	58.638	-10.887	25.321	1.00	56.28	N
ATOM	2702	CA	PRO	B	777	58.011	-9.569	25.464	1.00	55.27	C
ATOM	2703	CB	PRO	B	777	57.078	-9.548	24.271	1.00	55.36	C
ATOM	2704	CG	PRO	B	777	56.561	-10.950	24.291	1.00	56.03	C
ATOM	2705	CD	PRO	B	777	57.807	-11.793	24.508	1.00	56.21	C
ATOM	2706	C	PRO	B	777	57.189	-9.364	26.737	1.00	54.10	C
ATOM	2707	O	PRO	B	777	56.916	-10.338	27.466	1.00	53.82	O
ATOM	2708	N	THR	B	778	56.810	-8.103	26.983	1.00	52.28	N
ATOM	2709	CA	THR	B	778	55.960	-7.751	28.117	1.00	51.05	C
ATOM	2710	CB	THR	B	778	56.128	-6.263	28.526	1.00	51.62	C
ATOM	2711	OG1	THR	B	778	57.514	-5.930	28.693	1.00	52.75	O
ATOM	2712	CG2	THR	B	778	55.525	-6.018	29.916	1.00	51.07	C
ATOM	2713	C	THR	B	778	54.508	-7.973	27.702	1.00	49.65	C
ATOM	2714	O	THR	B	778	53.774	-7.020	27.460	1.00	49.64	O
ATOM	2715	N	LEU	B	779	54.098	-9.228	27.595	1.00	47.40	N
ATOM	2716	CA	LEU	B	779	52.748	-9.548	27.199	1.00	45.15	C
ATOM	2717	CB	LEU	B	779	52.486	-11.020	27.483	1.00	44.67	C
ATOM	2718	CG	LEU	B	779	53.553	-11.917	26.856	1.00	44.69	C
ATOM	2719	CD1	LEU	B	779	53.599	-13.324	27.488	1.00	45.78	C
ATOM	2720	CD2	LEU	B	779	53.361	-12.007	25.369	1.00	45.46	C
ATOM	2721	C	LEU	B	779	51.739	-8.680	27.941	1.00	44.03	C
ATOM	2722	O	LEU	B	779	51.867	-8.480	29.137	1.00	43.69	O
ATOM	2723	N	SER	B	780	50.729	-8.184	27.219	1.00	42.70	N
ATOM	2724	CA	SER	B	780	49.645	-7.367	27.780	1.00	41.09	C
ATOM	2725	CB	SER	B	780	48.967	-6.594	26.642	1.00	41.11	C
ATOM	2726	OG	SER	B	780	48.015	-5.655	27.119	1.00	41.62	O
ATOM	2727	C	SER	B	780	48.620	-8.238	28.496	1.00	40.22	C
ATOM	2728	O	SER	B	780	48.381	-9.353	28.080	1.00	39.24	O
ATOM	2729	N	PRO	B	781	47.997	-7.730	29.555	1.00	40.30	N
ATOM	2730	CA	PRO	B	781	47.066	-8.528	30.355	1.00	40.49	C
ATOM	2731	CB	PRO	B	781	46.795	-7.626	31.569	1.00	40.18	C
ATOM	2732	CG	PRO	B	781	46.953	-6.295	31.060	1.00	40.81	C
ATOM	2733	CD	PRO	B	781	48.136	-6.369	30.103	1.00	40.81	C

ATOM	2734	C	PRO	B	781	45.775	-8.859	29.620	1.00	40.94	C
ATOM	2735	O	PRO	B	781	45.134	-7.961	29.063	1.00	41.63	O
ATOM	2736	N	ILE	B	782	45.408	-10.140	29.606	1.00	40.96	N
ATOM	2737	CA	ILE	B	782	44.174	-10.590	28.961	1.00	41.15	C
ATOM	2738	CB	ILE	B	782	44.169	-12.125	28.886	1.00	41.28	C
ATOM	2739	CG1	ILE	B	782	45.321	-12.601	28.000	1.00	41.51	C
ATOM	2740	CD1	ILE	B	782	45.027	-12.473	26.509	1.00	42.88	C
ATOM	2741	CG2	ILE	B	782	42.817	-12.667	28.388	1.00	40.06	C
ATOM	2742	C	ILE	B	782	42.923	-10.093	29.710	1.00	41.48	C
ATOM	2743	O	ILE	B	782	42.915	-9.990	30.932	1.00	40.74	O
ATOM	2744	N	PRO	B	783	41.877	-9.749	28.967	1.00	41.74	N
ATOM	2745	CA	PRO	B	783	40.617	-9.334	29.579	1.00	42.10	C
ATOM	2746	CB	PRO	B	783	39.719	-9.080	28.374	1.00	41.64	C
ATOM	2747	CG	PRO	B	783	40.666	-8.777	27.311	1.00	41.40	C
ATOM	2748	CD	PRO	B	783	41.830	-9.692	27.497	1.00	41.11	C
ATOM	2749	C	PRO	B	783	40.049	-10.450	30.413	1.00	43.09	C
ATOM	2750	O	PRO	B	783	39.720	-11.490	29.879	1.00	42.35	O
ATOM	2751	N	HIS	B	784	39.907	-10.203	31.708	1.00	45.68	N
ATOM	2752	CA	HIS	B	784	39.388	-11.196	32.656	1.00	48.44	C
ATOM	2753	CB	HIS	B	784	38.831	-10.507	33.902	1.00	49.03	C
ATOM	2754	CG	HIS	B	784	38.870	-11.356	35.137	1.00	51.46	C
ATOM	2755	ND1	HIS	B	784	38.178	-12.545	35.248	1.00	53.83	N
ATOM	2756	CE1	HIS	B	784	38.390	-13.068	36.446	1.00	54.70	C
ATOM	2757	NE2	HIS	B	784	39.185	-12.254	37.122	1.00	54.84	N
ATOM	2758	CD2	HIS	B	784	39.506	-11.180	36.322	1.00	53.76	C
ATOM	2759	C	HIS	B	784	38.331	-12.109	32.048	1.00	49.08	C
ATOM	2760	O	HIS	B	784	38.559	-13.299	31.879	1.00	49.44	O
ATOM	2761	N	ILE	B	785	37.169	-11.552	31.746	1.00	50.08	N
ATOM	2762	CA	ILE	B	785	36.100	-12.296	31.075	1.00	51.26	C
ATOM	2763	CB	ILE	B	785	36.409	-12.469	29.563	1.00	51.67	C
ATOM	2764	CG1	ILE	B	785	35.162	-12.971	28.831	1.00	52.65	C
ATOM	2765	CD1	ILE	B	785	35.332	-13.007	27.347	1.00	54.35	C
ATOM	2766	CG2	ILE	B	785	37.583	-13.424	29.341	1.00	50.78	C
ATOM	2767	C	ILE	B	785	35.757	-13.651	31.643	1.00	51.63	C
ATOM	2768	O	ILE	B	785	35.905	-14.643	30.960	1.00	51.81	O
ATOM	2769	N	PRO	B	786	35.313	-13.691	32.890	1.00	52.49	N
ATOM	2770	CA	PRO	B	786	34.882	-14.933	33.536	1.00	52.77	C
ATOM	2771	CB	PRO	B	786	35.206	-14.656	34.998	1.00	52.72	C

ATOM	2772	CG	PRO	B	786	34.865	-13.198	35.163	1.00	52.87	C
ATOM	2773	CD	PRO	B	786	35.236	-12.542	33.817	1.00	53.07	C
ATOM	2774	C	PRO	B	786	33.381	-15.174	33.396	1.00	53.40	C
ATOM	2775	O	PRO	B	786	32.835	-15.085	32.279	1.00	53.92	O
ATOM	2776	N	ARG	B	787	32.730	-15.465	34.527	1.00	53.49	N
ATOM	2777	CA	ARG	B	787	31.274	-15.694	34.591	1.00	53.49	C
ATOM	2778	CB	ARG	B	787	30.480	-14.416	34.239	1.00	53.44	C
ATOM	2779	CG	ARG	B	787	30.063	-13.565	35.449	1.00	52.26	C
ATOM	2780	CD	ARG	B	787	31.223	-13.138	36.339	1.00	52.06	C
ATOM	2781	NE	ARG	B	787	30.807	-12.649	37.659	1.00	53.17	N
ATOM	2782	CZ	ARG	B	787	30.457	-13.428	38.706	1.00	51.86	C
ATOM	2783	NH1	ARG	B	787	30.468	-14.750	38.601	1.00	50.85	N
ATOM	2784	NH2	ARG	B	787	30.090	-12.880	39.864	1.00	49.91	N
ATOM	2785	C	ARG	B	787	30.800	-16.882	33.745	1.00	53.54	C
ATOM	2789	N	LEU	P	1	20.931	-14.544	31.252	1.00	47.69	N
ATOM	2790	CA	LEU	P	1	22.180	-13.716	31.289	1.00	47.41	C
ATOM	2791	CB	LEU	P	1	23.030	-14.044	32.535	1.00	47.97	C
ATOM	2792	CG	LEU	P	1	23.458	-15.482	32.878	1.00	48.35	C
ATOM	2793	CD1	LEU	P	1	24.423	-15.489	34.063	1.00	49.77	C
ATOM	2794	CD2	LEU	P	1	22.266	-16.389	33.165	1.00	48.66	C
ATOM	2795	C	LEU	P	1	22.987	-13.883	29.991	1.00	46.60	C
ATOM	2796	O	LEU	P	1	22.417	-13.727	28.897	1.00	47.13	O
ATOM	2797	N	ASP	P	2	24.287	-14.207	30.109	1.00	44.53	N
ATOM	2798	CA	ASP	P	2	25.177	-14.357	28.935	1.00	42.24	C
ATOM	2799	CB	ASP	P	2	24.541	-15.300	27.910	1.00	42.69	C
ATOM	2800	CG	ASP	P	2	25.522	-15.772	26.866	1.00	44.51	C
ATOM	2801	OD1	ASP	P	2	25.766	-15.024	25.896	1.00	45.50	O
ATOM	2802	OD2	ASP	P	2	26.093	-16.887	26.932	1.00	46.89	O
ATOM	2803	C	ASP	P	2	25.516	-12.983	28.288	1.00	39.49	C
ATOM	2804	O	ASP	P	2	26.077	-12.893	27.200	1.00	39.39	O
ATOM	2805	N	TYR	P	3	25.145	-11.911	28.970	1.00	35.91	N
ATOM	2806	CA	TYR	P	3	25.408	-10.565	28.477	1.00	32.30	C
ATOM	2807	CB	TYR	P	3	24.129	-9.724	28.549	1.00	31.47	C
ATOM	2808	CG	TYR	P	3	24.334	-8.262	28.269	1.00	31.00	C
ATOM	2809	CD1	TYR	P	3	24.418	-7.805	26.965	1.00	29.48	C
ATOM	2810	CE1	TYR	P	3	24.583	-6.478	26.693	1.00	27.36	C
ATOM	2811	CZ	TYR	P	3	24.676	-5.570	27.712	1.00	27.68	C
ATOM	2812	OH	TYR	P	3	24.888	-4.218	27.370	1.00	28.65	O

ATOM	2813	CE2	TYR	P	3	24.582	-5.991	29.034	1.00	25.24	C
ATOM	2814	CD2	TYR	P	3	24.407	-7.315	29.309	1.00	27.91	C
ATOM	2815	C	TYR	P	3	26.471	-10.014	29.386	1.00	29.47	C
ATOM	2816	O	TYR	P	3	26.400	-10.230	30.588	1.00	28.95	O
ATOM	2817	N	HIS	P	4	27.456	-9.330	28.820	1.00	26.50	N
ATOM	2818	CA	HIS	P	4	28.564	-8.759	29.600	1.00	24.52	C
ATOM	2819	CB	HIS	P	4	29.803	-8.571	28.690	1.00	24.64	C
ATOM	2820	CG	HIS	P	4	30.980	-7.912	29.349	1.00	25.77	C
ATOM	2821	ND1	HIS	P	4	31.453	-8.268	30.598	1.00	30.26	N
ATOM	2822	CE1	HIS	P	4	32.496	-7.522	30.917	1.00	27.94	C
ATOM	2823	NE2	HIS	P	4	32.732	-6.707	29.910	1.00	26.64	N
ATOM	2824	CD2	HIS	P	4	31.790	-6.919	28.926	1.00	27.32	C
ATOM	2825	C	HIS	P	4	28.197	-7.412	30.271	1.00	22.87	C
ATOM	2826	O	HIS	P	4	28.058	-6.414	29.595	1.00	21.47	O
ATOM	2827	N	PHE	P	5	28.025	-7.405	31.590	1.00	21.22	N
ATOM	2828	CA	PHE	P	5	27.773	-6.153	32.298	1.00	20.74	C
ATOM	2829	CB	PHE	P	5	26.881	-6.357	33.494	1.00	18.47	C
ATOM	2830	CG	PHE	P	5	25.501	-6.754	33.152	1.00	16.23	C
ATOM	2831	CD1	PHE	P	5	25.193	-8.091	32.917	1.00	14.97	C
ATOM	2832	CE1	PHE	P	5	23.887	-8.475	32.631	1.00	13.89	C
ATOM	2833	CZ	PHE	P	5	22.881	-7.505	32.578	1.00	11.09	C
ATOM	2834	CE2	PHE	P	5	23.182	-6.167	32.806	1.00	10.80	C
ATOM	2835	CD2	PHE	P	5	24.471	-5.790	33.087	1.00	11.98	C
ATOM	2836	C	PHE	P	5	29.109	-5.609	32.769	1.00	21.26	C
ATOM	2837	O	PHE	P	5	29.724	-6.195	33.664	1.00	21.67	O
ATOM	2838	N	GLY	P	6	29.556	-4.502	32.170	1.00	21.32	N
ATOM	2839	CA	GLY	P	6	30.859	-3.926	32.468	1.00	21.51	C
ATOM	2840	C	GLY	P	6	30.831	-2.897	33.585	1.00	22.19	C
ATOM	2841	O	GLY	P	6	31.865	-2.528	34.114	1.00	21.62	O
ATOM	2842	N	LEU	P	7	29.651	-2.406	33.919	1.00	23.30	N
ATOM	2843	CA	LEU	P	7	29.543	-1.497	35.032	1.00	25.46	C
ATOM	2844	CB	LEU	P	7	28.154	-0.859	35.099	1.00	25.82	C
ATOM	2845	CG	LEU	P	7	27.814	0.211	34.061	1.00	26.11	C
ATOM	2846	CD1	LEU	P	7	26.339	0.562	34.191	1.00	24.70	C
ATOM	2847	CD2	LEU	P	7	28.709	1.422	34.234	1.00	21.99	C
ATOM	2848	C	LEU	P	7	29.817	-2.254	36.323	1.00	26.52	C
ATOM	2849	O	LEU	P	7	29.437	-3.421	36.472	1.00	25.30	O
ATOM	2850	N	GLU	P	8	30.492	-1.567	37.240	1.00	28.49	N

ATOM	2851	CA	GLU	P	8	30.779	-2.099	38.551	1.00	31.21	C
ATOM	2852	CB	GLU	P	8	32.215	-1.763	38.887	1.00	32.54	C
ATOM	2853	CG	GLU	P	8	33.179	-2.369	37.881	1.00	38.33	C
ATOM	2854	CD	GLU	P	8	34.639	-2.164	38.254	1.00	44.38	C
ATOM	2855	OE1	GLU	P	8	34.977	-1.015	38.639	1.00	47.15	O
ATOM	2856	OE2	GLU	P	8	35.437	-3.145	38.151	1.00	44.55	O
ATOM	2857	C	GLU	P	8	29.830	-1.509	39.593	1.00	30.87	C
ATOM	2858	O	GLU	P	8	29.277	-0.443	39.374	1.00	30.40	O
ATOM	2859	N	GLU	P	9	29.655	-2.193	40.726	1.00	31.54	N
ATOM	2860	CA	GLU	P	9	28.722	-1.742	41.790	1.00	31.59	C
ATOM	2861	CB	GLU	P	9	28.841	-2.607	43.057	1.00	32.17	C
ATOM	2862	CG	GLU	P	9	28.217	-4.028	42.934	1.00	34.26	C
ATOM	2863	CD	GLU	P	9	28.018	-4.747	44.294	1.00	33.72	C
ATOM	2864	OE1	GLU	P	9	27.685	-4.084	45.314	1.00	33.47	O
ATOM	2865	OE2	GLU	P	9	28.185	-5.978	44.350	1.00	31.42	O
ATOM	2866	C	GLU	P	9	28.826	-0.254	42.133	1.00	30.99	C
ATOM	2867	O	GLU	P	9	27.826	0.429	42.361	1.00	31.00	O
ATOM	2868	N	GLY	P	10	30.033	0.276	42.153	1.00	30.01	N
ATOM	2869	CA	GLY	P	10	30.155	1.696	42.418	1.00	29.07	C
ATOM	2870	C	GLY	P	10	29.895	2.598	41.209	1.00	27.90	C
ATOM	2871	O	GLY	P	10	30.205	3.806	41.240	1.00	28.51	O
ATOM	2872	N	GLU	P	11	29.353	2.024	40.138	1.00	25.73	N
ATOM	2873	CA	GLU	P	11	29.073	2.791	38.922	1.00	23.64	C
ATOM	2874	CB	GLU	P	11	29.952	2.303	37.748	1.00	24.46	C
ATOM	2875	CG	GLU	P	11	31.459	2.612	37.875	1.00	26.02	C
ATOM	2876	CD	GLU	P	11	32.325	1.859	36.852	1.00	26.65	C
ATOM	2877	OE1	GLU	P	11	33.486	2.296	36.631	1.00	24.35	O
ATOM	2878	OE2	GLU	P	11	31.853	0.824	36.281	1.00	26.05	O
ATOM	2879	C	GLU	P	11	27.603	2.753	38.516	1.00	21.13	C
ATOM	2880	O	GLU	P	11	26.905	1.758	38.653	1.00	19.86	O
ATOM	2881	N	GLY	P	12	27.131	3.855	38.005	1.00	19.40	N
ATOM	2882	CA	GLY	P	12	25.766	3.895	37.535	1.00	18.44	C
ATOM	2883	C	GLY	P	12	25.582	4.880	36.401	1.00	17.74	C
ATOM	2884	O	GLY	P	12	26.404	5.785	36.161	1.00	16.52	O
ATOM	2885	N	ILE	P	13	24.458	4.734	35.719	1.00	17.35	N
ATOM	2886	CA	ILE	P	13	24.156	5.570	34.567	1.00	17.40	C
ATOM	2887	CB	ILE	P	13	22.680	5.451	34.230	1.00	16.80	C
ATOM	2888	CG1	ILE	P	13	22.353	6.275	32.979	1.00	17.71	C

ATOM	2889	CD1	ILE	P	13	23.048	5.763	31.684	1.00	18.51	C
ATOM	2890	CG2	ILE	P	13	21.913	5.983	35.380	1.00	17.44	C
ATOM	2891	C	ILE	P	13	24.535	7.051	34.805	1.00	17.29	C
ATOM	2892	O	ILE	P	13	24.899	7.769	33.896	1.00	17.49	O
ATOM	2893	N	ARG	P	14	24.443	7.527	36.022	1.00	16.45	N
ATOM	2894	CA	ARG	P	14	24.749	8.917	36.228	1.00	17.18	C
ATOM	2895	CB	ARG	P	14	24.232	9.313	37.598	1.00	17.84	C
ATOM	2896	CG	ARG	P	14	24.580	10.693	38.068	1.00	17.51	C
ATOM	2897	CD	ARG	P	14	25.712	10.655	39.027	1.00	19.60	C
ATOM	2898	NE	ARG	P	14	25.496	11.615	40.079	1.00	21.69	N
ATOM	2899	CZ	ARG	P	14	26.127	11.610	41.237	1.00	22.46	C
ATOM	2900	NH1	ARG	P	14	27.038	10.683	41.515	1.00	20.71	N
ATOM	2901	NH2	ARG	P	14	25.840	12.557	42.113	1.00	22.29	N
ATOM	2902	C	ARG	P	14	26.228	9.319	36.051	1.00	17.89	C
ATOM	2903	O	ARG	P	14	26.533	10.465	35.749	1.00	18.28	O
ATOM	2904	N	ASP	P	15	27.153	8.388	36.249	1.00	17.97	N
ATOM	2905	CA	ASP	P	15	28.557	8.678	36.058	1.00	17.42	C
ATOM	2906	CB	ASP	P	15	29.419	7.620	36.731	1.00	17.17	C
ATOM	2907	CG	ASP	P	15	28.943	7.257	38.136	1.00	16.85	C
ATOM	2908	OD1	ASP	P	15	28.567	8.168	38.917	1.00	14.72	O
ATOM	2909	OD2	ASP	P	15	28.933	6.068	38.549	1.00	17.21	O
ATOM	2910	C	ASP	P	15	28.893	8.700	34.576	1.00	18.51	C
ATOM	2911	O	ASP	P	15	29.888	9.266	34.154	1.00	19.86	O
ATOM	2912	N	LEU	P	16	28.067	8.078	33.752	1.00	19.15	N
ATOM	2913	CA	LEU	P	16	28.383	8.009	32.351	1.00	19.27	C
ATOM	2914	CB	LEU	P	16	27.482	7.006	31.674	1.00	19.48	C
ATOM	2915	CG	LEU	P	16	27.817	5.590	32.121	1.00	18.49	C
ATOM	2916	CD1	LEU	P	16	26.903	4.583	31.531	1.00	16.38	C
ATOM	2917	CD2	LEU	P	16	29.205	5.334	31.714	1.00	18.61	C
ATOM	2918	C	LEU	P	16	28.287	9.373	31.691	1.00	20.34	C
ATOM	2919	O	LEU	P	16	28.964	9.619	30.688	1.00	18.95	O
ATOM	2920	N	PHE	P	17	27.423	10.216	32.264	1.00	22.07	N
ATOM	2921	CA	PHE	P	17	27.160	11.583	31.843	1.00	24.13	C
ATOM	2922	CB	PHE	P	17	25.668	11.799	31.553	1.00	23.78	C
ATOM	2923	CG	PHE	P	17	25.128	10.936	30.490	1.00	22.61	C
ATOM	2924	CD1	PHE	P	17	24.659	9.689	30.789	1.00	21.60	C
ATOM	2925	CE1	PHE	P	17	24.142	8.878	29.790	1.00	22.90	C
ATOM	2926	CZ	PHE	P	17	24.160	9.321	28.432	1.00	24.90	C

ATOM	2927	CE2	PHE	P	17	24.662	10.542	28.122	1.00	23.17	C
ATOM	2928	CD2	PHE	P	17	25.144	11.351	29.158	1.00	24.24	C
ATOM	2929	C	PHE	P	17	27.470	12.403	33.045	1.00	26.26	C
ATOM	2930	O	PHE	P	17	26.583	13.079	33.582	1.00	26.70	O
ATOM	2931	N	ASP	P	18	28.717	12.312	33.505	1.00	29.15	N
ATOM	2932	CA	ASP	P	18	29.152	12.999	34.732	1.00	31.05	C
ATOM	2933	CB	ASP	P	18	29.110	12.033	35.922	1.00	31.59	C
ATOM	2934	CG	ASP	P	18	29.079	12.741	37.254	1.00	35.19	C
ATOM	2935	OD1	ASP	P	18	29.132	12.001	38.293	1.00	37.21	O
ATOM	2936	OD2	ASP	P	18	29.007	14.012	37.355	1.00	37.60	O
ATOM	2937	C	ASP	P	18	30.566	13.540	34.586	1.00	31.76	C

Claims

1. A crystal structure of the pRb/E2F$_{(409-426)}$ complex, characterised by the atomic co-ordinates of Annex 1.

2. A crystal structure as claimed in claim 1, wherein the interactions between E2F$_{(409-426)}$ and pRb comprise one or more of the following interactions:

E2F$_{(409-426)}$ residue	pRb residue
Leu_{409}	Lys_{548}
Tyr_{411}	Glu_{551}
Tyr_{411}	Ile_{532}
Tyr_{411}	Glu_{554}
His_{412}	Arg_{656}
His_{412}	Lys_{653}
Gly_{414}	Glu_{533}
Gly_{414}	Lys_{652}
Leu_{415}	Leu_{649}
Leu_{415}	Glu_{553}
Leu_{415}	Lys_{537}
Glu_{417}	Lys_{537}
Gly_{418}	Arg_{467}
Glu_{419}	Thr_{645}
Arg_{422}	Glu_{464}
Asp_{423}	Arg_{467}
Leu_{424}	Lys_{530}
Phe_{425}	Phe_{482}
Phe_{425}	Lys_{475}

3. A method to identify an agent which modulates the interaction between pRb and $E2F_{(409-426)}$, the method comprising:

a) combining together pRb, $E2F_{(409-426)}$ and an agent, under conditions in which pRb and $E2F_{(409-426)}$ form a complex;

b) growing a crystal structure of any pRb/ $E2F_{(409-426)}$ complex; and

c) analysing the crystal to determine whether the agent is an agent which modulates the interaction between pRb and $E2F_{(409-426)}$.

4. A method, as claimed in claim 3, wherein the combining of the components is pRb with the agent and then $E2F_{(409-426)}$.

5. A method as claimed in claim 3, wherein the combining of the components is $E2F_{(409-426)}$ with the agent and then pRb.

6. A method as claimed in claim 3, wherein the combining of the components is pRb with $E2F_{(409-426)}$ and then the agent.

7. A method as claimed in any one of claims 3 to 6, wherein step c) comprises comparing the crystal structure to the crystal structure of claim 1

8. A method as claimed in any one of claims 3 to 7, wherein the agent is selected using the three dimensional atomic co-ordinates of Annex 1.

9. A method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising selecting an agent using the three-dimensional atomic coordinates of Annex 1.

10. A method as claimed in claim 9, wherein said selection is performed in conjunction with computer modeling.

11. A method as claimed in claim 9 or 10, wherein the method further comprises the steps of:

a) contacting the selected agent with pRb and $E2F_{(409-426)}$ under conditions in which pRb and $E2F_{(409-426)}$ can form a complex; and

b) measuring the binding affinity of pRb to $E2F_{(409-426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to $E2F_{(409-426)}$ when in the absence of the agent, wherein an agent modulates a pRb/$E2F_{(409-426)}$ complex when there is a change in the binding affinity of pRb to $E2F_{(409-426)}$ when in the presence of the agent.

12. A method as claimed in claim 11, wherein the method further comprising:

a) growing a supplementary crystal from a solution containing pRb and $E2F_{(409-426)}$ and the selected agent where said agent changes the binding affinity of the pRb/$E2F_{(409-426)}$ complex under conditions in which pRb and $E2F_{(409-426)}$ can form a complex;

b) determining the three-dimensional atomic coordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;

c) comparing the three dimensional coordinates with those for the crystal structure as claimed in claim 1; and

d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal.

13. A method as claimed in claim 12, wherein said selection is performed in conjunction with computer modeling.

14. A method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising:

a) contacting a selected agent with pRb and $E2F_{(409-426)}$ under conditions in which pRb and $E2F_{(409-426)}$ can form a complex; and

b) measuring the binding affinity of pRb to $E2F_{(409-426)}$ in the presence of the agent and comparing the binding affinity to that of pRb to $E2F_{(409-426)}$ when in the absence of the agent, wherein an agent modulates a pRb/$E2F_{(409-426)}$ complex when there is a change in the binding affinity of pRb to $E2F_{(409-426)}$ when in the presence of the agent.

15. A method as claimed in claim 14, wherein the method further comprising:

a) growing a supplementary crystal from a solution containing pRb and $E2F_{(409-426)}$ and the selected agent where said agent changes the binding affinity of the pRb/$E2F_{(409-426)}$ complex under conditions in which pRb and $E2F_{(409-426)}$ can form a complex;

b) determining the three-dimensional atomic coordinates of the supplementary crystal by X-ray diffraction using molecular replacement analysis;

c) comparing the three dimensional coordinates with those for the crystal structure claimed in claim 1; and

d) selecting a second generation agent using the three-dimensional atomic coordinates determined for the supplementary crystal.

16. A method as claimed in claim 15, wherein said selection is performed in conjunction with computer modeling.

17. A method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising:

a) selecting an agent;

b) co-crystalising pRb with the agent;

c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and

d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

18. A method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) crystalising pRb and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

19. A method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb, E2F$_{(409-426)}$ and the agent;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

20. A method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising:

a) selecting an agent;
b) co-crystalising pRb and E2F$_{(409-426)}$ and soaking the agent into the crystal;
c) determining the three dimensional coordinates of the pRb-E2F-agent association by X-ray diffraction using molecular replacement analysis; and
d) comparing the three dimensional coordinates with those of the crystal structure claimed in claim 1.

21. A method as claimed in any one of claims 17 to 20, wherein the agent is selected using the three dimensional atomic co-ordinates of Annex 1

22. A method as claimed in any one of claims 17 to 21, wherein the methods further comprise selecting a second generation agent using the three dimensional atomic coordinates determined in step c).

23. A method as claimed in claim 22, wherein the second generation agent is selected using the three dimensional atomic coordinates of Annex 1.

24. A method as claimed in claim 22 or 23, wherein the selection is performed in conjunction with computer modeling.

25. A method of identifying an agent as claimed in any one of claims 3 to 24, wherein the selected agent and/or the second generation agent mimics a structural feature of $E2F_{(409-426)}$, when said $E2F_{(409-426)}$ is bound to pRb.

26. A method as claimed in claim 9 or 10, wherein method comprises the further steps of:

a) contacting the selected agent with a pRb/$E2F_{(409-426)}$ complex; and
b) determining whether the agent affects the stability of the complex.

27. A method as claimed in claim 26, wherein the determination is with fluorescence polarization.

28. A method of identifying an agent that modulates a pRb/$E2F_{(409-426)}$ complex, comprising:

a) contacting a fluorescently tagged $E2F_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;
b) detecting the fluorescence polarization;

c) adding a selected agent; and

d) detecting the fluorescence polarization in the presence of the agent.

29. A method of identifying an agent that modulates a pRb/E2F$_{(409-426)}$ complex, comprising;

a) contacting a fluorescently tagged E2F$_{(409-426)}$ peptide (E2F-fluoropeptide) with pRb to allow pRb/E2F-fluoropeptide complex formation;

b) detecting the fluorescence polarization;

c) contacting a selected agent with pRb and E2F$_{(409-426)}$ peptide (E2F-fluoropeptide) under conditions in which pRb and E2F-fluoropeptide can form a complex;

d) detecting the fluorescence polarization; and

e) comparing the fluorescence polarization detected in b) and d).

30. A method as claimed in claim 28 or 29, wherein the fluorescently tagged E2F peptide is selected using the three dimensional atomic co-ordinates of Annex 1.

31. A method as claimed in any one of claims 28 to 30, wherein a decrease in fluorescence polarization in the presence of the agent indicates that the agent destabilises the complex.

32. A method as claimed in any one of claims 28 to 31, wherein the method comprises the further step of adding untagged E2F$_{(409-426)}$ and detecting fluorescence polarization.

33. A method as claimed in claim 32, wherein if fluorescence polarization decreases, on addition of the untagged E2F$_{(409-426)}$, the agent does not stabilise the complex.

34. A method as claimed in claim 32 or 33, wherein if there is no substantial change in fluorescence polarization, on addition of the untagged E2F$_{(409-426)}$, the agent stabilises the complex.

35. A method as claimed in any one of claims 28 to 34, wherein the method further comprises:

a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) adding an agent that modulates pRb/E2F$_{(409\text{-}426)}$ complex; and
d) detecting the fluorescence polarization in the presence of the agent.

36. A method as claimed in any one of claims 28 to 34, wherein the method further comprises:

a) contacting a fluorescently tagged E7 peptide (E7-fluoropeptide) with pRb to allow pRb/E7-fluoropeptide complex formation;
b) detecting the fluorescence polarization;
c) contacting an agent that modulates pRb/E2F$_{(409\text{-}426)}$ complex with pRb and E7-fluoropeptide under conditions in which pRb and E7-fluoropeptide can from a complex;
d) detecting the fluorescence polarization; and
e) comparing the fluorescence polarization detected in b) and d).

37. A method as claimed in claim 35 or 36, wherein a decrease in fluorescence polarization indicates that the agent also inhibits E7 binding to pRb.

38. A method as claimed in any one of claims 11 to 16, wherein the binding affinity is measured by isothermal titration calorimetry.

39. A method as claimed in any one of claims 11 to 16, wherein the binding affinity is measure by Surface Plasmon Resonance (SPR).

40. An agent, that modulates the interaction between pRb and $E2F_{(409-426)}$, identified by a method as claimed in any one of claims 3 to 39.

41. An agent, as claimed in claim 40, for use as an apoptosis promoting factor in the prevention or treatment of proliferative diseases.

42. An agent as claimed in claim 40 or 41, wherein the agent is for use in preventing or treating cancer, which may be pancreatic cancer and related diseases.

43. The use of an agent, which modulates the formation of a $pRb/E2F_{(409-426)}$ complex, identified by a method as claimed in any one of claims 3 to 39, in the manufacture of a medicament for the prevention or treatment of proliferative diseases.

44. The use of an agent as claimed in claim 43, wherein the proliferative diseases are cancer, preferably pancreatic cancer and related diseases.

45. The use of the atomic co-ordinates of the crystal structure as claimed in claim 1 or 2, for identifying an agent that modulates the formation of a $pRb/E2F_{(409-426)}$ complex.

46. Computer readable media comprising a data storage material encoded with computer readable data, wherein said computer readable data comprises a set of atomic co-ordinates of the $pRb/E2F_{(409-426)}$ crystal structure of Annex 1 recorded thereon.

FIG. 1A

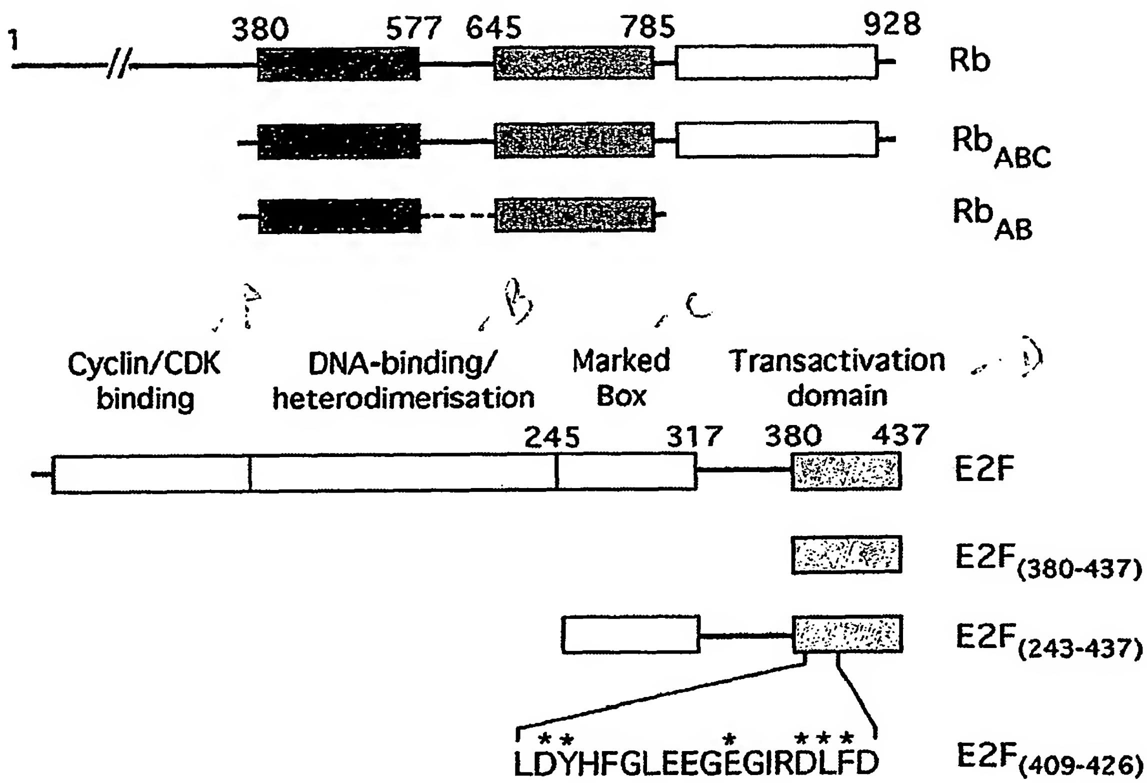

1
380
577
645
785
928
Rb
Rb ABC
Rb AB
A
B
C
D
Cyclin/CDK binding
DNA-binding/ heterodimerisation
Marked Box
Transactivation domain
245
317
380
437
E2F
E2F(380-437)
E2F(243-437)
LDYHFGLEEGEGIRDLFD
E2F(409-426)

FIG. 1B

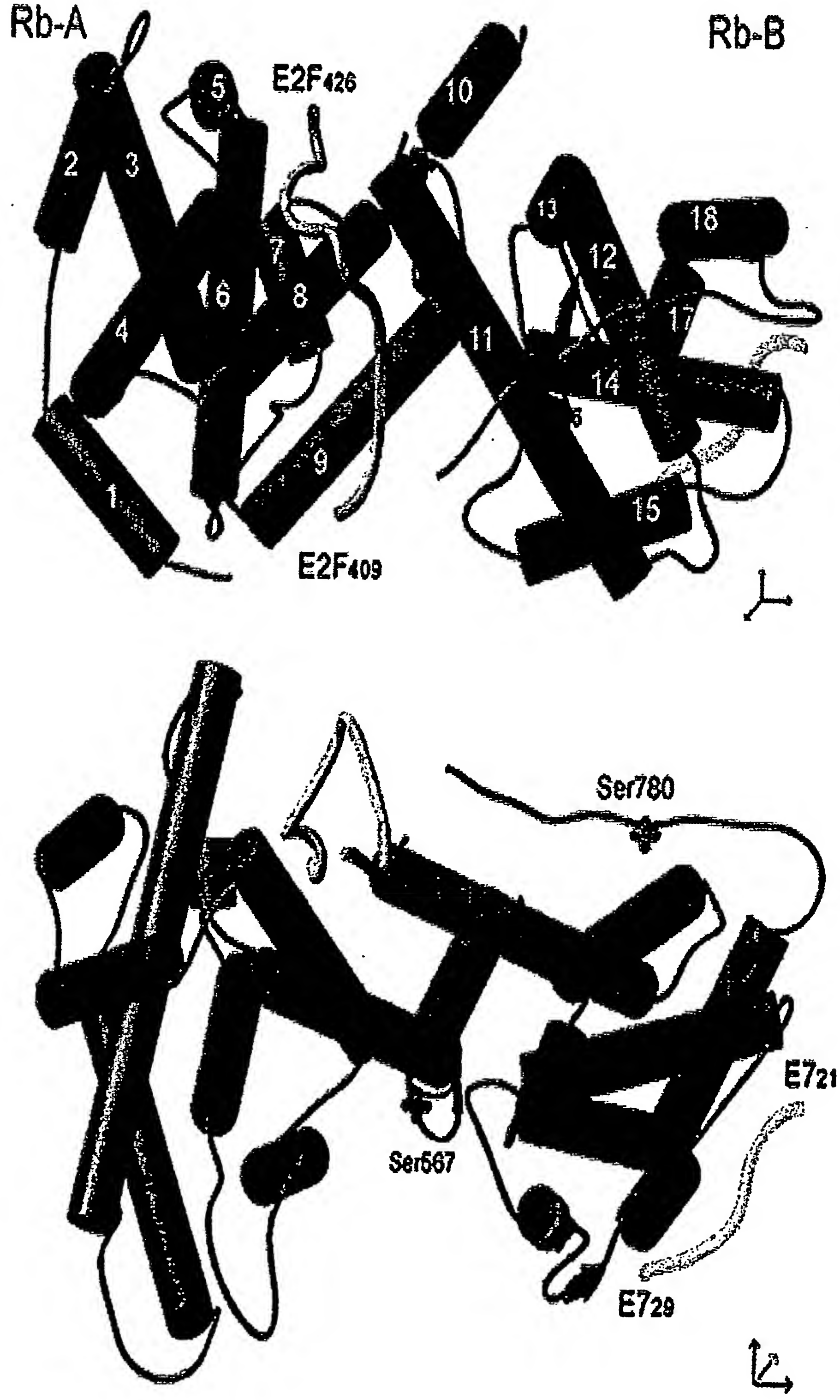

Rb-A
Rb-B
E2F426
E2F409
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
Ser780
Ser567
E721
E729

FIG. 1C

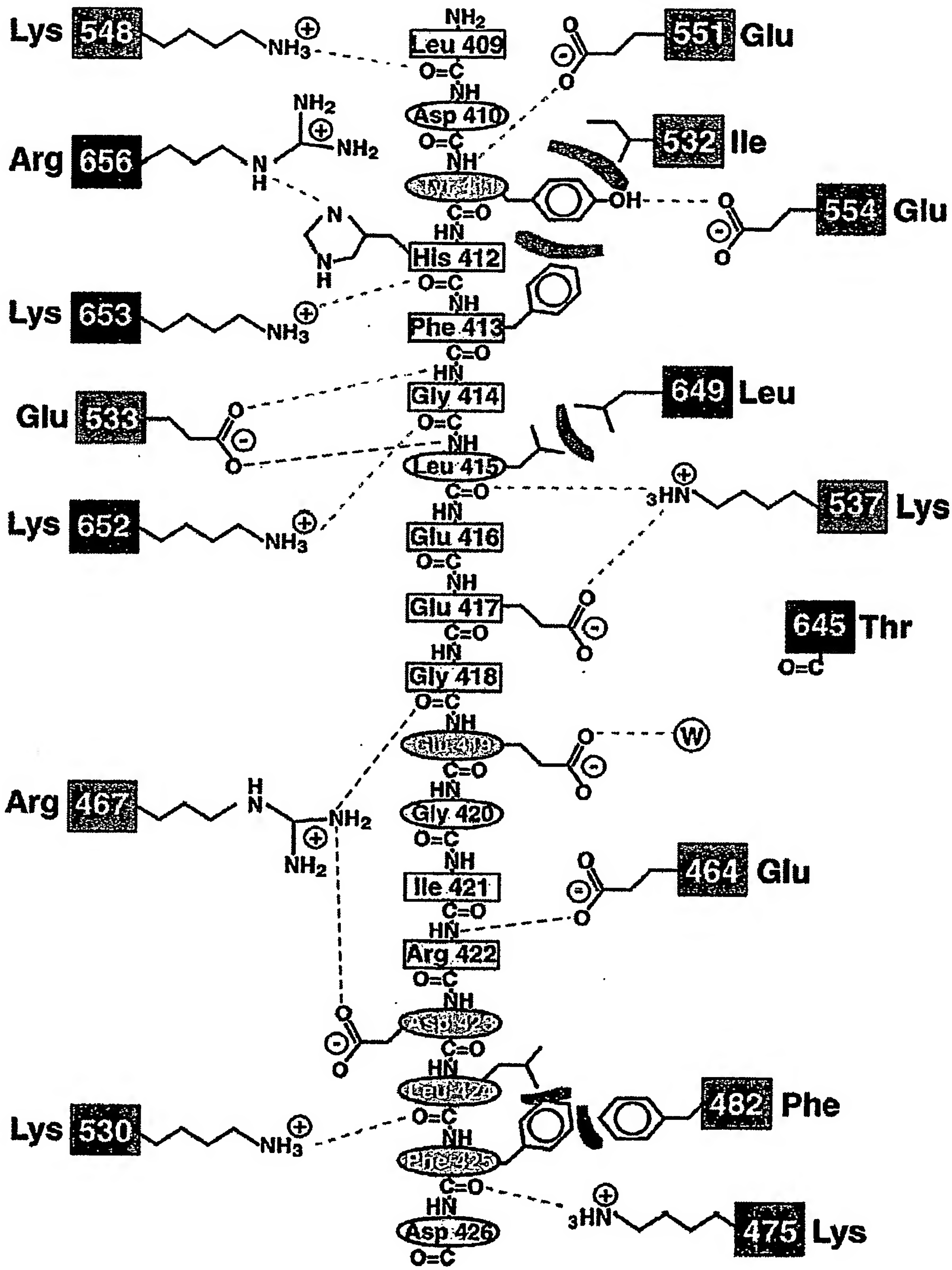

Lys 548
Leu 409
551 Glu
Asp 410
Arg 656
532 Ile
554 Glu
His 412
Lys 653
Phe 413
Gly 414
649 Leu
Glu 533
Leu 415
537 Lys
Lys 652
Glu 416
Glu 417
645 Thr
Gly 418
W
Arg 467
Gly 420
Ile 421
464 Glu
Arg 422
Lys 530
482 Phe
475 Lys
Asp 426

FIG. 2A

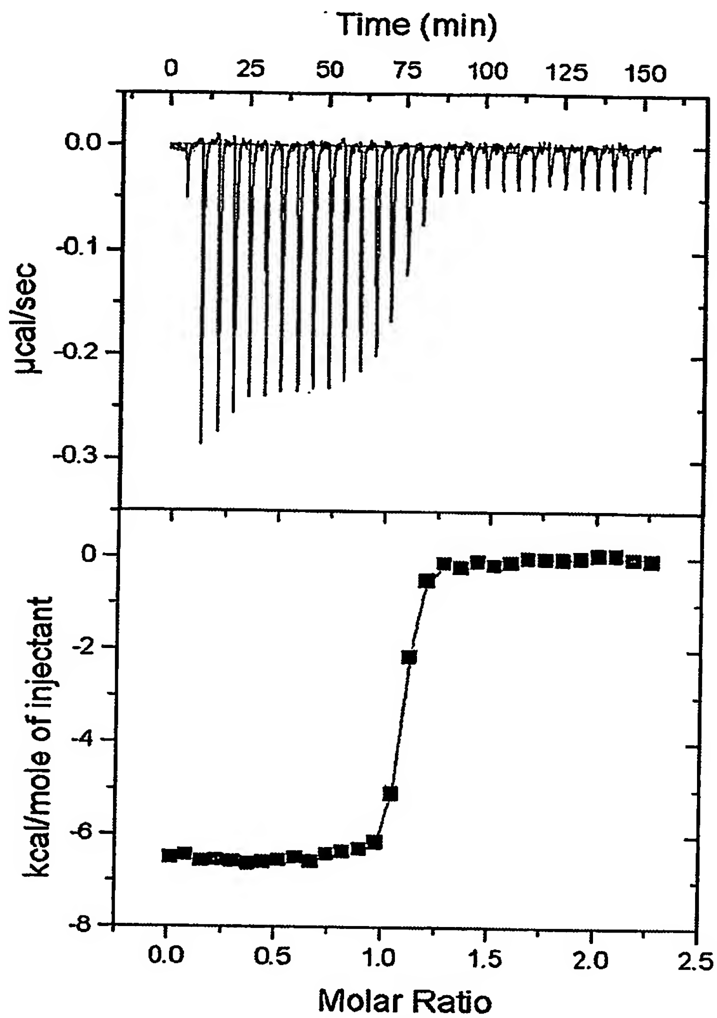


FIG. 2B

Binding Constants (µM)	Rb_{AB}	Rb_{ABC}
E2F (409-426)	0.34±0.02	0.3±0.03
E2F (380-437)	0.16±0.01	0.1±0.01
E2F (243-437)	<0.01	<0.01

FIG. 3

Binding of Fluorescein-E2F, Rhodamine-E2F and Fluorescein-E7 to pRb

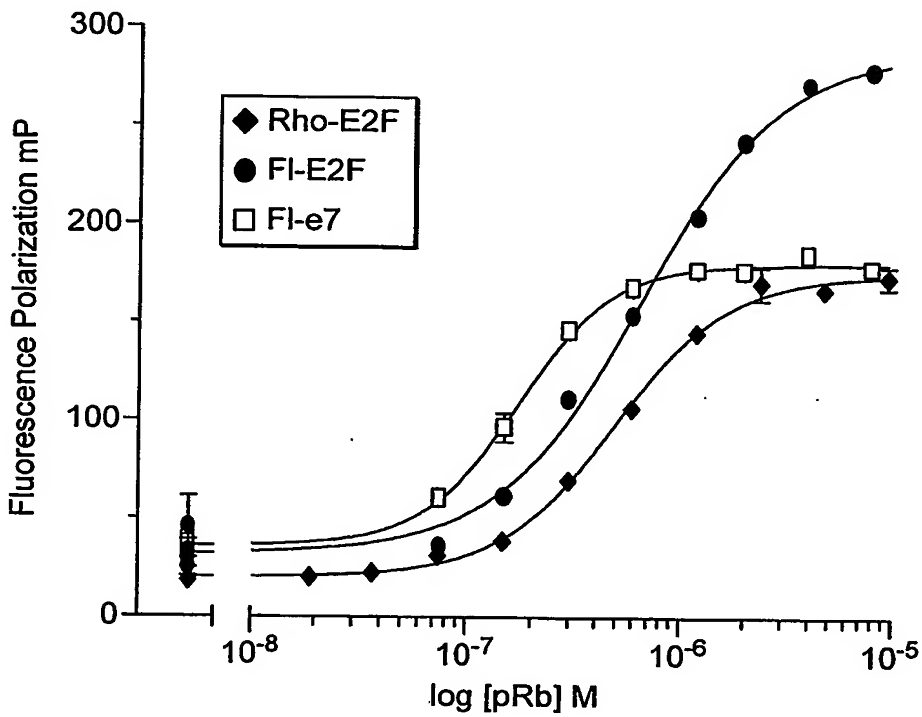
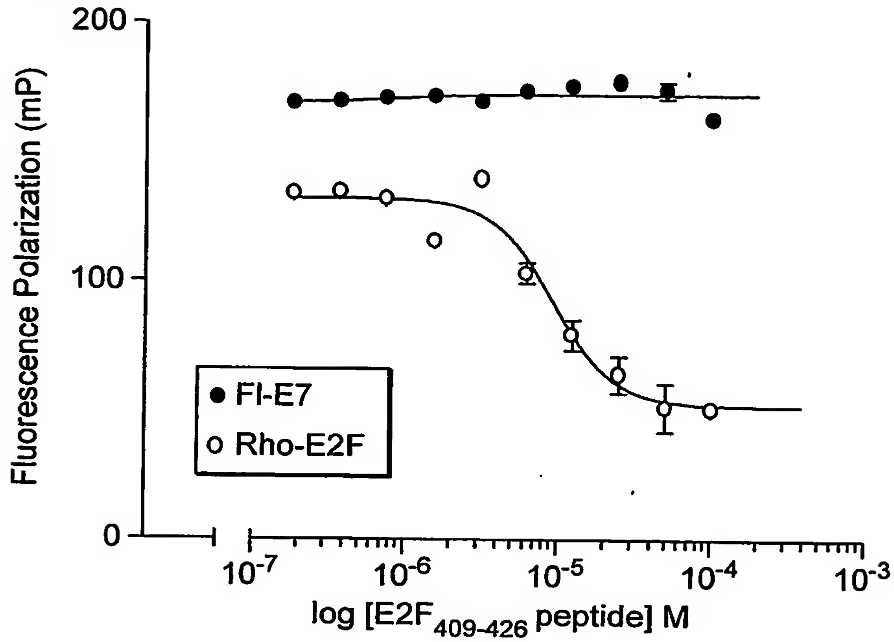


FIG. 4

Displacement Binding Curves

(a)



(b)

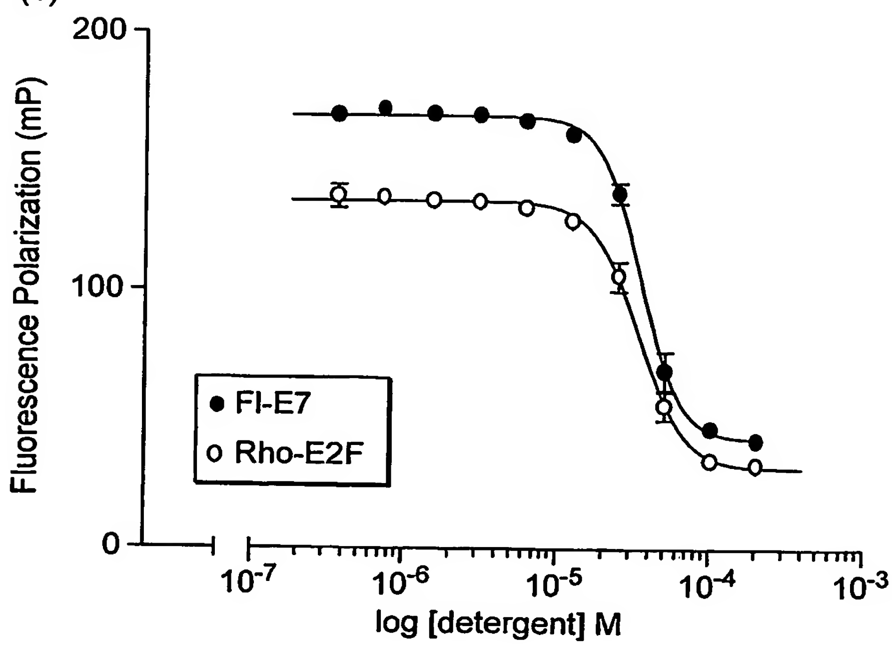


FIG. 5

Screen controls from Test Screen 6X384 plates

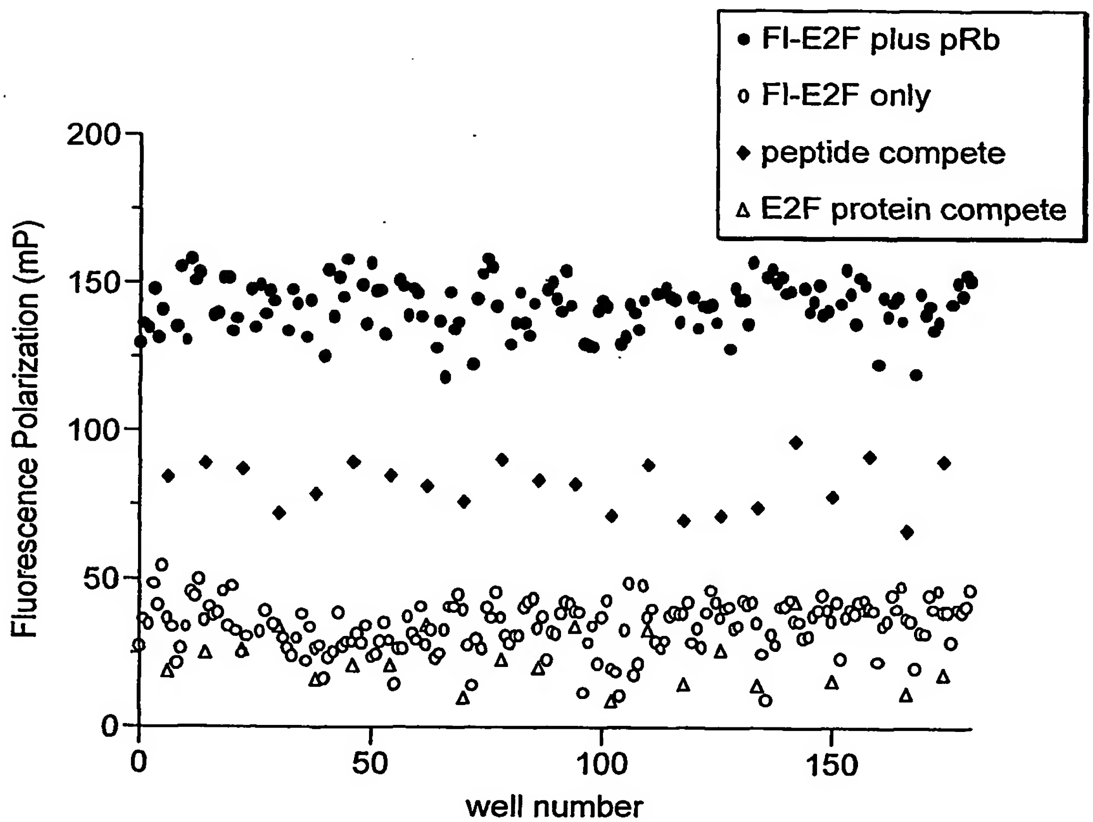


FIG. 6

Correlation Inhibition Rhodamine and Fluorescein-E2F

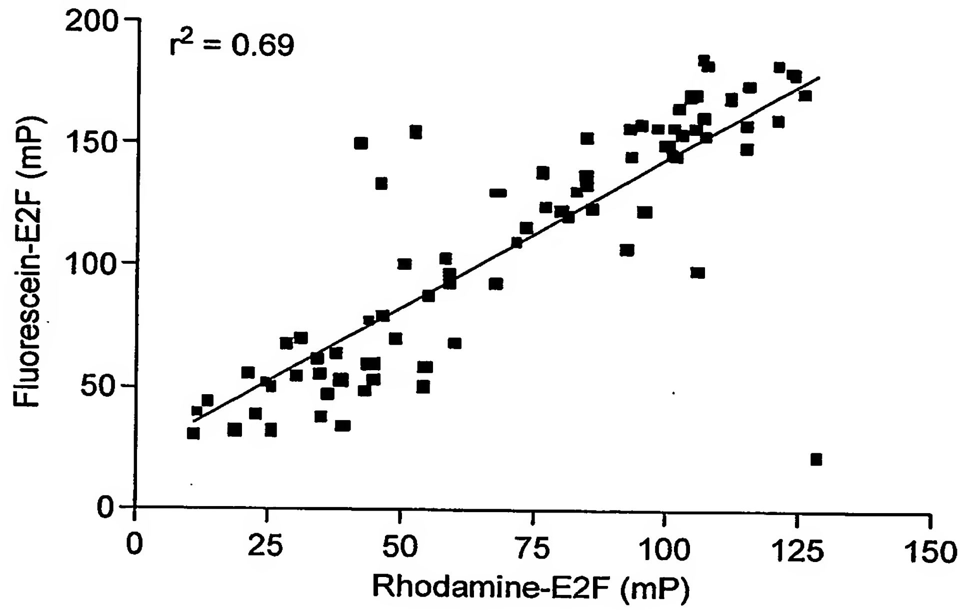


FIG. 7

Correlation Inhibition Fluorescein-E2F and Fluorescein-E7

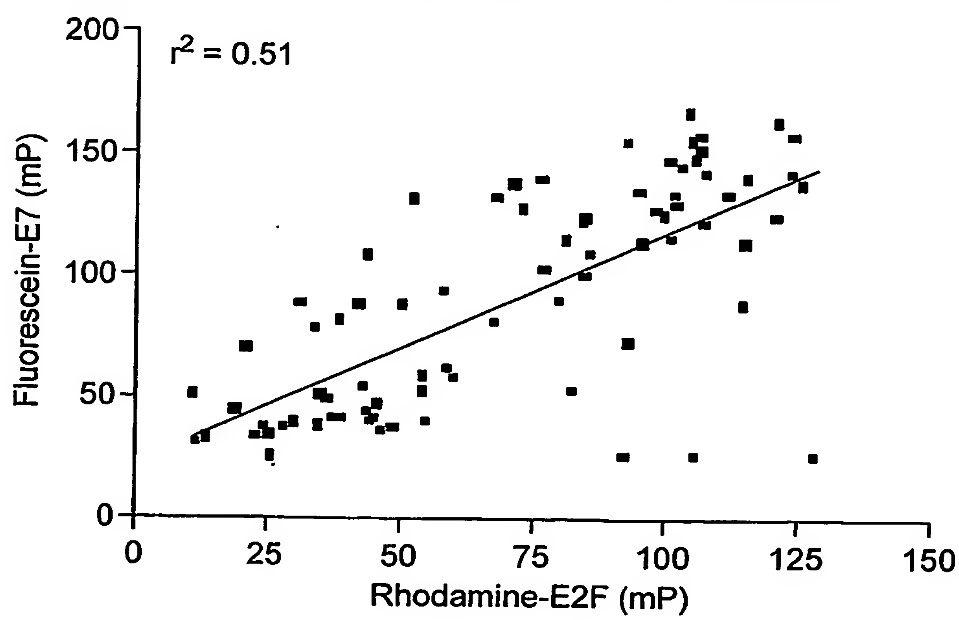
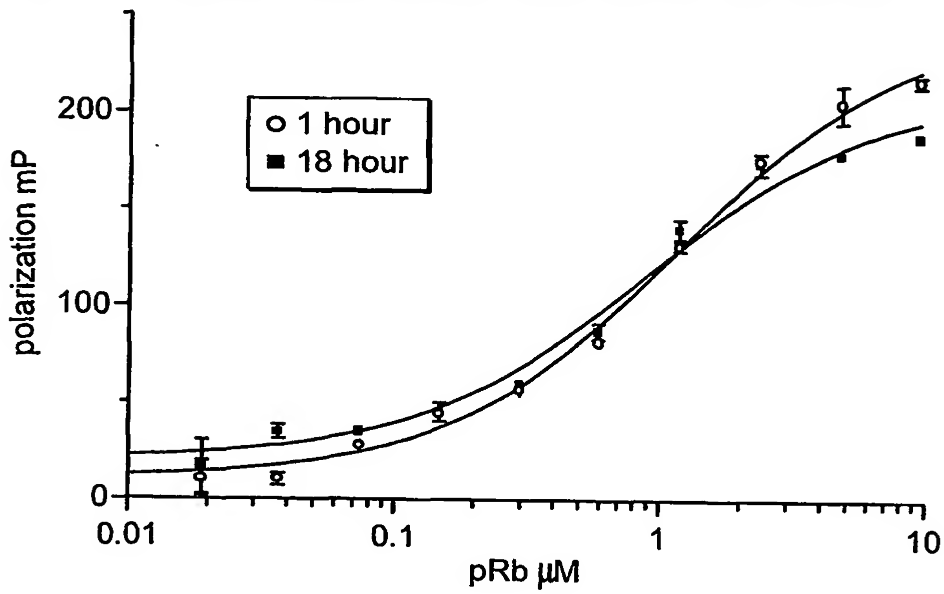


FIG. 8

(a) peptide titration curves measured at 1 and 18 hour



(b) Time course peptide binding

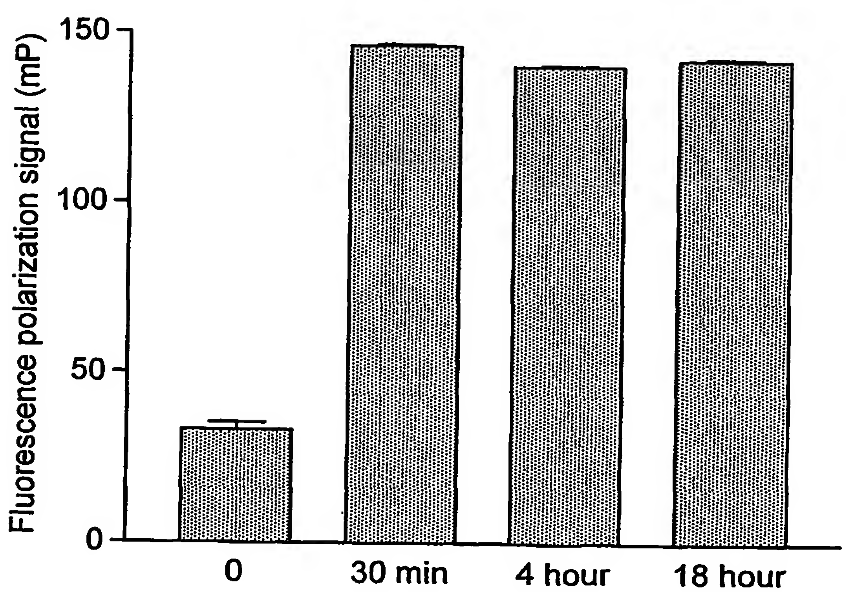
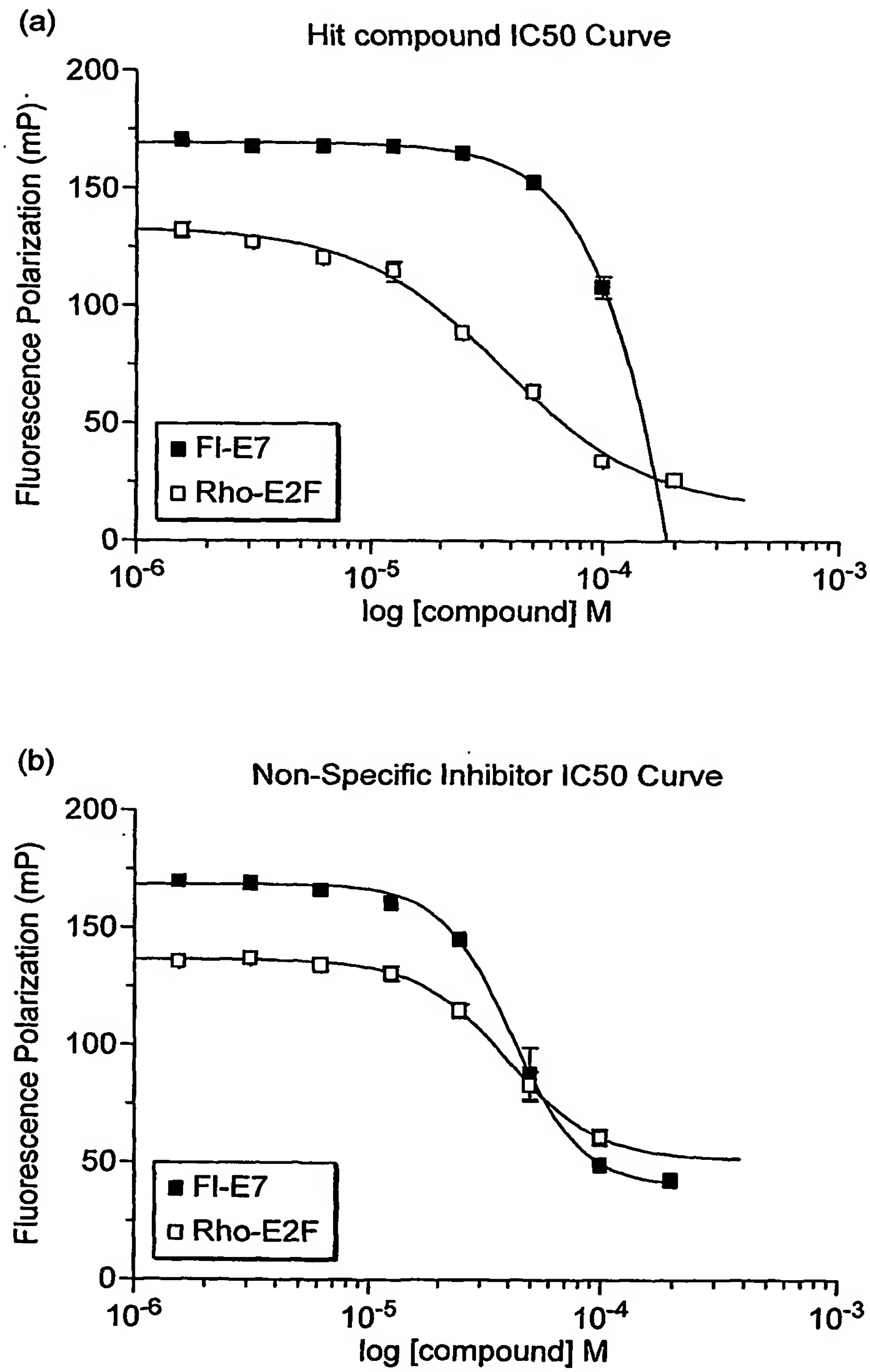


FIG. 9


(a)
Hit compound IC50 Curve
Fluorescence Polarization (mP)
200
150
100
50
0
FI-E7
Rho-E2F
10^{-6}
10^{-5}
10^{-4}
10^{-3}
log [compound] M
(b)
Non-Specific Inhibitor IC50 Curve
Fluorescence Polarization (mP)
200
150
100
50
0
FI-E7
Rho-E2F
10^{-6}
10^{-5}
10^{-4}
10^{-3}
log [compound] M

# INTERNATION[redacted]SEARCH REPORT	Internat[redacted]Application No PCT/[redacted]3/05158

A. CLASSIFICATION OF SUBJECT MA[redacted]R
IPC 7 C07K14/47

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

BIOSIS, EPO-Internal, MEDLINE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	LEE JIE-OH ET AL: "Structure of the retinoblastoma tumour-suppressor pocket domain bound to a peptide from HPV E7" NATURE (LONDON), vol. 391, no. 6670, 26 February 1998 (1998-02-26), pages 859-865, XP002272473 ISSN: 0028-0836 the whole document ---	3-39,45
Y	HELIN K ET AL: "A CDNA ENCODING A PRB-BINDING PROTEIN WITH PROPERTIES OF THE TRANSCRIPTION FACTOR E2F" CELL, CELL PRESS, CAMBRIDGE, NA, US, vol. 70, no. 2, 24 July 1992 (1992-07-24), pages 337-350, XP000872846 ISSN: 0092-8674 the whole document --- -/--	3-39,45

[X] Further documents are listed in the continuation of box C.

[ ] Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
14 April 2004	22/04/2004

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Wimmer, G

C.(Continuation) DOCUMENTS CONSID[redacted]D TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	DATABASE PDB 'Online! RCSB; 7 January 2003 (2003-01-07) LEE CHANGWOOK ET AL: "Structure of rb tumor suppressor bound to the transactivation domain of e2f-2" retrieved from PDB Database accession no. 1n4m XP002272474 the whole document & LEE CHANGWOOK ET AL: "Structural basis for the recognition of the E2F transactivation domain by the retinoblastoma tumor suppressor." GENES & DEVELOPMENT. UNITED STATES 15 DEC 2002, vol. 16, no. 24, 15 December 2002 (2002-12-15), pages 3199-3212, ISSN: 0890-9369 ---	3-39,45
P,X	DATABASE PDB 'Online! RCSB; 6 March 2003 (2003-03-06) XIAO ET AL: "Crystal Structure Of The Retinoblastoma Tumour Suppressor Protein Bound To E2F Peptide" retrieved from PDB Database accession no. 1o9k XP002272475 abstract & XIAO ET AL.: "Crystal Structure of the Retinoblastoma Tumor" PROC.NATL.ACAD.SCI., vol. 100, no. 5, 21 February 2003 (2003-02-21), pages 2363-2368, USA -----	3-39,45

INTERNATION[redacted]EARCH REPORT	Inter[redacted]lication No. PC[redacted] 03/05158

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims Nos.: 1, 2, 46
because they relate to subject matter not required to be searched by this Authority, namely:
Rule 39.1(v) PCT - Presentation of information

2. [X] Claims Nos.: 40-44
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
see FURTHER INFORMATION sheet PCT/ISA/210

3. [ ] Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2. [ ] As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

4. [ ] No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

[ ] The additional search fees were accompanied by the applicant's protest.

[ ] No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 40-44

Present claims 40-44 relate to compounds defined by reference to a desirable characteristic or property, namely that they modulate the interaction between pRb and E2F, and that they may be identified by one of the claimed in silico sceening or modeling methods.

The claims cover all compounds having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for no such compounds. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the compounds by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, no search has been carried out for these claims.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.